Close

Web of Science
Page 1 (Records 1 -- 50)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 1 of 491

Title: Raman antenna effect from exciton-phonon coupling in organic semiconducting nanobelts

Author(s): Wang, M (Wang, Mao); Gong, Y (Gong, Yi); Alzina, F (Alzina, Francesc); Svoboda, O (Svoboda, Ondrej); Ballesteros, B (Ballesteros, Belen); Torres, CMS (Sotomayor Torres, Clivia M.); Xiao, SB (Xiao, Senbo); Zhang, ZL (Zhang, Zhiliang); He, JY (He, Jianying)

Source: NANOSCALE **Volume:** 9 **Issue:** 48 **Pages:** 19328-19336 **DOI:** 10.1039/c7nr07212k **Published:** DEC 28 2017

Abstract: The highly anisotropic interactions in organic semiconductors together with the soft character of organic materials lead to strong coupling between nuclear vibrations and exciton dynamics, which potentially results in anomalous electrical, optical and optoelectrical properties. Here, we report on the Raman antenna effect from organic semiconducting nanobelts 6,13-dichloropentacene (DCP), resulting from the coupling of molecular excitons and intramolecular phonons. The highly ordered crystalline structure in DCP nanobelts enables the precise polarization-resolved spectroscopic measurement. The angle-dependent Raman spectroscopy under resonant excitation shows that all Raman modes from the skeletal vibrations of DCP molecule act like a nearly perfect dipole antenna I-Raman proportional to cos(4)(theta - 90), with almost zero (maximum) Raman scattering parallel (perpendicular) to the nanobelt's long-axis. The Raman antenna effect in DCP nanobelt is originated from the coupling between molecular skeletal vibrations and intramolecular exciton and the confinement of intermolecular excitons. It dramatically enhances the Raman polarization ratio (rho = I-parallel to/I-perpendicular to > 25) and amplifies the anisotropy of the angle-dependent Raman scattering (kappa(Raman) = I-max/I-min > 12) of DCP nanobelts. These findings have crucial implications for fundamental understanding on the exciton-phonon coupling and its effects on the optical properties of organic semiconductors.

Accession Number: WOS:000418098000039

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ballesteros, Belen	B-1167-2010	0000-0002-1958-8911
Alzina, Francesc	C-5468-2008	0000-0002-7082-0624
He, Jianying	C-8747-2009	0000-0001-8485-7893
Sotomayor Torres, Clivia	E-8418-2010	0000-0001-9986-2716
		0000-0002-9557-3455

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Record 2 of 491

Title: Spin-orbit driven phenomena in the isoelectronic L1(0)-Fe(Pd,Pt) alloys from first principles

Author(s): Kudrnovsky, J (Kudrnovsky, J.); Drchal, V (Drchal, V.); Turek, I (Turek, I.)

Source: PHYSICAL REVIEW B **Volume:** 96 **Issue:** 21 **Article Number:** 214437 **DOI:** 10.1103/PhysRevB.96.214437 **Published:** DEC 26 2017

Abstract: The anomalous Hall effect (AHE) and the Gilbert damping (GD) are studied theoretically for the partially ordered L1(0)-Fe(Pd,Pt) alloys. The varying alloy order and the spin-orbit coupling, which are due to the change in the Pd/Pt composition, allow for a chemical tuning of both phenomena which play an important role in the spintronic applications. The impact of the antisite disorder on the residual resistivity, AHE, and GD is studied from first principles using recently developed methods employing the Kubo-Bastin approach and the nonlocal torque operator method. The most interesting result is a different behavior of samples with low and high chemical orders. Good agreement between calculated and measured concentration trends is obtained for all quantities studied, while the absolute GD values are underestimated.

Accession Number: WOS:000418653000009

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Turek, Ilja	G-5553-2014	0000-0002-0604-6590

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Record 3 of 491

Title: The benchmark of P-31 NMR parameters in phosphate: a case study on structurally constrained and flexible phosphate

Author(s): Fukal, J (Fukal, Jiri); Pav, O (Pav, Ondrej); Budesinsky, M (Budesinsky, Milos); Sebera, J (Sebera, Jakub); Sychrovsky, V (Sychrovsky, Vladimir)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 47 **Pages:** 31830-31841 **DOI:** 10.1039/c7cp06969c **Published:** DEC 21 2017

Abstract: A benchmark for structural interpretation of the P-31 NMR shift and the (2)J(P),(C) NMR spin-spin coupling in the phosphate group was obtained by means of theoretical calculations and NMR measurements in diethylphosphate (DEP) and 5,5-dimethyl-2-hydroxy-1,3,2-dioxaphosphinane 2-oxide (cDEP). The NMR parameters were calculated employing the B3LYP, BP86, BPW91, M06-2X, PBE0, KT2, KT3, MP2, and HF methods, and the 6-31+G(d), Iglo-n (n = II, III), cc-pVnZ (n = D, T, Q, 5), aug-cc-pVnZ (n = D, T and Q), and pcS-n and pcJ-n (n = 1, 2, 3, 4) bases, including the solvent effects described with explicit water molecules and/or the implicit Polarizable Continuum Model (PCM). The effect of molecular dynamics (MD) on NMR parameters was MD-calculated using the GAFF force field inclusive of explicit hydration with TIP3P water molecules. Both the optimal geometries and the dynamic behaviors of the DEP and cDEP phosphates differed notably, which allowed a reliable theoretical benchmark of the P-31 NMR parameters for highly flexible and structurally constrained phosphate in a one-to-one relationship with the corresponding experiment. The calculated P-31 NMR shifts were referenced employing three different NMR reference schemes to highlight the effect of the P-31 NMR reference on the accuracy of the calculated P-31 NMR shift. The relative Dd(P-31) NMR shift calculated employing the MD/B3LYP/Iglo-III/PCM method differed from the experiment by 0.16 ppm while the NMR shifts referenced to H3PO4 and/or PH3 deviated from the experiment notably more, which illustrated the superior applicability of the relative NMR reference scheme. The (2)J(P,C) coupling in DEP and cDEP calculated employing theMD/B3LYP/Iglo-III(DSO,PSO,SD)/cc-PV5Z(FC)/PCM method inclusive of correction due to explicit hydration differed from the experiment by 0.32 Hz and 0.15 Hz, respectively. The NMR calculations demonstrated that reliable structural interpretation of the P-31 NMR parameters in phosphate must involve both the structural and the dynamical components.

Accession Number: WOS:000417295800034

PubMed ID: 29171602

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sebera, Jakub	B-6112-2013	0000-0001-5671-5206

ISSN: 1463-9076

eISSN: 1463-9084

Record 4 of 491

Title: Chiral ethylene-bridged flavinium salts: the stereoselectivity of flavin-10a-hydroperoxide formation and the effect of substitution on the photochemical properties

Author(s): Zurek, J (Zurek, Jiri); Svobodova, E (Svobodova, Eva); Sturala, J (Sturala, Jiri); Dvorakova, H (Dvorakova, Hana); Svoboda, J (Svoboda, Jiri); Cibulka, R (Cibulka, Radek)

Source: TETRAHEDRON-ASYMMETRY **Volume:** 28 **Issue:** 12 **Pages:** 1780-1791 **DOI:** 10.1016/j.tetasy.2017.10.029 **Published:** DEC 15 2017

Abstract: A series of chiral non-racemic N-1,N-10-ethylene bridged flavinium salts 4 was prepared using enantiomerically pure 2-substituted 2-aminoethanols (R = isopropyl, phenyl, benzyl, 4-methoxybenzyl, 4-benzyloxybenzyl) derived from amino acids as the sole source of chirality. The flavinium salts were shown to form 10a-hydroperoxy- and 10a-methoxy-adducts with moderate to high diastereoselectivity depending on the ethylene bridge substituent originating from the starting amino acid. High diastereoselectivities (dr values from 80:20 to >95:5) were observed for flavinium salts bearing benzyl substituents attached to the ethylene bridge. The benzyl group preferred the face-to-face (syn) orientation relative to the flavinium unit; thereby effectively preventing nucleophilic attack from one side. This conformation was found to be the most stable according to the DFT calculations. Consequently, the presence of benzyl groups causes intermolecular fluorescence quenching resulting in a significant decrease in the fluorescence quantum yield from 11% for 4a bearing an isopropyl substituent to 0.3% for 4c containing a benzyl group and to a value lower than 0.1% for the benzyloxybenzyl derivative 4e. (C) 2017 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000418988400014

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sturala, Jiri		0000-0002-8113-0709

ISSN: 0957-4166

Record 5 of 491

Title: Unexpected Crystallization Patterns of Zinc Boron Imidazolate Framework ZBIF-1: NMR Crystallography of Integrated Metal-Organic Frameworks

Author(s): Kobera, L (Kobera, Libor); Rohlicek, J (Rohlicek, Jan); Czernek, J (Czernek, Jiri); Abbrent, S (Abbrent, Sabina); Streckova, M (Streckova, Magdalena); Sopcak, T (Sopcak, Tibor); Brus, J (Brus, Jiri)

Source: CHEMPHYSCHEM **Volume:** 18 **Issue:** 24 **Pages:** 3576-3582 **DOI:** 10.1002/cphc.201701063 **Published:** DEC 15 2017

Abstract: Framework materials, that is, metal-organic frameworks (MOFs) and inorganic frameworks (zeolites), are porous systems with regular structures that provide valuable properties suitable for sorption, catalysis, molecular sieving, and so on. Herein, an efficient, experimental/computational strategy is presented that allows detailed characterization of a polycrystalline MOF system, namely, zinc boron imidazolate framework ZBIF-1, with two integrated unit cells on the atomic-resolution level. Although high-resolution H-1, B-11, C-13, and N-15 MAS NMR spectra provide valuable structural information on the coexistence of two distinct asymmetric units in the investigated system, an NMR crystallography approach combining X-ray powder diffraction, solid-state NMR spectroscopy, and DFT calculations allowed the exact structure of the secondary crystalline phase to be firmly defined and, furthermore, the mutual interconnectivity of the two crystalline frameworks to be resolved. Thus, this study shows the versatility and efficiency of solid-state NMR crystallography for the investigation of the wide family of MOF materials with their extensive structural complexity.

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PubMed ID: 29048717

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kobera, Libor	G-5237-2014	0000-0002-8826-948X
Brus, Jiri	G-3459-2014	
Abbrent, Sabina	M-9812-2014	
Czernek, Jiri	H-6708-2014	

ISSN: 1439-4235

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Record 6 of 491

Title: Role of spin-orbit interaction on the nonlinear optical response of CsPbCO3F using DFT

Author(s): Rao, EN (Rao, E. Narsimha); Vaitheeswaran, G (Vaitheeswaran, G.); Reshak, AH (Reshak, Ali H.); Auluck, S (Auluck, S.)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 46 **Pages:** 31255-31266 **DOI:** 10.1039/c7cp05750d **Published:** DEC 14 2017

Abstract: We explore the effect of spin-orbit interaction (SOI) on the electronic and optical properties of CsPbCO3F using the full potential Linear augmented Wane wave method with the density functional theory (DFT) approach. CsPbCO3F is known for its high powder second harmonic generation (SHG) coefficient (13.4 times (d(36) = 0.39 pm V-1) that of KH2PO4 (KDP)). Calculations are done for many exchange correlation (XC) potentials. After the inclusion of SOI, the calculated Tran-Eilaha modified Becke-Johnson (TB-mBJ) band gap of 5.58 eV reduces to 4.45 eV in agreement with the experimental value. This is due to the splitting of Pb p-states. Importantly, the occurrence of a band gap along the H-A direction (indirect) transforms to the H-H (direct) high symmetry points/direction in the first BriRouin zone. We noticed a Large anisotropy in the calculated complex dielectric function, absorption, and refractive index spectra. The calculated static birefringence of 0.1049 and 0.1057 (with SOI) is found to be higher than that of the other carbonate fluorides. From the Born effective charge (BEC) analysis we notice that the Cs atom shows a negative contribution to birefringence whereas Pb, C, and F atoms show a positive contribution. In addition, we have also calculated the nonlinear optical chi((2))(ijk)(2 omega;omega,omega) dispersion of a CsPbCO3F single crystal. We found that d(11) = d(12) = 4.35 pm V-1 at 1064 nm, which is 11.2 times higher than d(36) of KDP. The origin of the highly nonlinear optical susceptibility dispersion of CsPbCO3F is explained. Overall, our results are in agreement with experiments and it is obvious from the present study that CsPbCO3F is a direct band gap, Large second harmonic generation, and good phase matchable NLO crystal in the ultraviolet region.

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PubMed ID: 29147697

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363

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Record 7 of 491

Title: Excited-State Aromatic Interactions in the Aggregation-Induced Emission of Molecular Rotors

Author(s): Sturala, J (Sturala, Jiri); Etherington, MK (Etherington, Marc K.); Bismillah, AN (Bismillah, Aisha N.); Higginbotham, HF (Higginbotham, Heather F.); Trewby, W (Trewby, William); Aguilar, JA (Aguilar, Juan A.); Bromley, EHC (Bromley, Elizabeth H. C.); Avestro, AJ (Avestro, Alyssa-Jennifer); Monkman, AP (Monkman, Andrew P.); McGonigal, PR (McGonigal, Paul R.)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 139 **Issue:** 49 **Pages:** 17882-17889 **DOI:** 10.1021/jacs.7b08570 **Published:** DEC 13 2017

Abstract: Small, apolar aromatic groups, such as phenyl rings, are commonly included in the structures of fluorophores to impart hindered intramolecular rotations, leading to.desirable solid-state luminescence properties. However, they are not normally considered to take part in through-space interactions that influence the fluorescent output. Here, we report on the photoluminescence properties of a series of phenyl-ring molecular rotors bearing three, five, six, and seven phenyl groups. The fluorescent emissions from two of the rotors are found to originate, not from the localized excited state as one might expect, but from unanticipated through-space aromatic-dimer states. We demonstrate that these relaxed dimer states can form as a result of intra- or intermolecular interactions across a range of environments in solution and solid samples, including conditions that promote aggregation-induced emission. Computational modeling also suggests that the formation of aromatic-dimer excited states may account for the photophysical properties of a previously reported luminogen. These results imply, therefore, that this is a general phenomenon that should be taken into account when designing and interpreting the fluorescent outputs of luminescent probes and optoelectronic devices based on fluorescent molecular rotors.

Accession Number: WOS:000418204600034

Author Identifiers:

Author	ResearcherID Number	ORCID Number
McGonigal, Paul	J-8291-2012	0000-0002-8538-7579
Etherington, Marc Kenneth		0000-0003-2101-5757
Sturala, Jiri		0000-0002-8113-0709

ISSN: 0002-7863

Record 8 of 491

Title: A novel type I cystatin of parasite origin with atypical legumain-binding domain

Author(s): Ilgova, J (Ilgova, Jana); Jedlickova, L (Jedlickova, Lucie); Dvorakova, H (Dvorakova, Hana); Benovics, M (Benovics, Michal); Mikes, L (Mikes, Libor); Janda, L (Janda, Lubomir); Vorel, J (Vorel, Jiri); Roudnicky, P (Roudnicky, Pavel); Potesil, D (Potesil, David); Zdrahal, Z (Zdrahal, Zbynek); Gelnar, M (Gelnar, Milan); Kasny, M (Kasny, Martin)

Source: SCIENTIFIC REPORTS **Volume:** 7 **Article Number:** 17526 **DOI:** 10.1038/s41598-017-17598-2 **Published:** DEC 13 2017

Abstract: Parasite inhibitors of cysteine peptidases are known to influence a vast range of processes linked to a degradation of either the parasites' own proteins or proteins native to their hosts. We characterise a novel type I cystatin (stefin) found in a sanguinivorous fish parasite Eudiplozoon nipponicum (Platyhelminthes: Monogenea). We have identified a transcript of its coding gene in the transcriptome of adult worms. Its amino acid sequence is similar to other stefins except for containing a legumain-binding domain, which is in this type of cystatins rather unusual. As expected, the recombinant form of E. nipponicum stefin (rEnStef) produced in Escherichia coli inhibits clan CA peptidases - cathepsins L and B of the worm - via the standard papain-binding domain. It also blocks haemoglobinolysis by cysteine peptidases in the worm's excretory-secretory products and soluble extracts. Furthermore, we had confirmed its ability to inhibit clan CD asparaginyl endopeptidase (legumain). The presence of a native EnStef in the excretory-secretory products of adult

worms, detected by mass spectrometry, suggests that this protein has an important biological function at the host-parasite interface. We discuss the inhibitor's possible role in the regulation of blood digestion, modulation of antigen presentation, and in the regeneration of host tissues.

Accession Number: WOS:000417796000046

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vorel, Jiri		0000-0001-9106-6440

ISSN: 2045-2322

Record 9 of 491

Title: Influence of Trp flipping on carbohydrate binding in lectins. An example on Aleuria aurantia lectin AAL

Author(s): Houser, J (Houser, Josef); Kozmon, S (Kozmon, Stanislav); Mishra, D (Mishra, Deepti); Mishra, SK (Mishra, Sushi K.); Romano, PR (Romano, Patrick R.); Wimmerova, M (Wimmerova, Michaels); Koca, J (Koca, Jaroslav)

Source: PLOS ONE **Volume:** 12 **Issue:** 12 **Article Number:** e0189375 **DOI:** 10.1371/journal.pone.0189375 **Published:** DEC 12 2017

Abstract: Protein-carbohydrate interactions are very often mediated by the stacking CH-pi interactions involving the side chains of aromatic amino acids such as tryptophan (Trp), tyrosine (Tyr) or phenylalanine (Phe). Especially suitable for stacking is the Trp residue. Analysis of the PDB database shows Trp stacking for 265 carbohydrate or carbohydrate like ligands in 5 208 Trp containing motives. An appropriate model system to study such an interaction is the AAL lectin family where the stacking interactions play a crucial role and are thought to be a driving force for carbohydrate binding. In this study we present data showing a novel finding in the stacking interaction of the AAL Trp side chain with the carbohydrate. High resolution X-ray structure of the AAL lectin from Aleuria aurantia with alpha-methyl-L-fucoside ligand shows two possible Trp side chain conformations with the same occupation in electron density. The in silico data shows that the conformation of the Trp side chain does not influence the interaction energy despite the fact that each conformation creates interactions with different carbohydrate CH groups. Moreover, the PDB data search shows that the conformations are almost equally distributed across all Trp-carbohydrate complexes, which would suggest no substantial preference for one conformation over another.

Accession Number: WOS:000417698200036

PubMed ID: 29232414

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houser, Josef	D-7319-2012	0000-0003-4504-3891
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Wimmerova, Michaela		0000-0002-7108-4198

ISSN: 1932-6203

Record 10 of 491

Title: Lithium borate Li3B5O8(OH)(2) with large second harmonic generation and a high damage threshold in the deep-ultraviolet spectral range

Author(s): Reshak, AH (Reshak, A. H.)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 45 **Pages:** 30703-30714 **DOI:** 10.1039/c7cp06006h **Published:** DEC 7 2017

Abstract: The electronic structure and linear and nonlinear optical susceptibility dispersions of lithium borate Li3B5O8(OH)(2) are comprehensively investigated. The investigation is achieved on Li3B5O8(OH)(2) in the form of single crystals, taking into account the influence of the packing of the structural units on the linear and nonlinear optical susceptibility dispersion. The calculations highlight that the BO3 structural unit packing is the main source of the large birefringence in Li3B5O8(OH)(2) due to the high anisotropic electron distribution, and, hence, it affects the macroscopic second harmonic generation (SHG) coefficients. This work provides a new path for the design of UV-NLO materials with high SHG efficiencies and short cutoff edges by introducing an alkali metal into borates. The large SHG is due to hyperpolarizability formed by co-parallel BO3 triangle groups. The absorption edge of Li3B5O8(OH)(2) occurs at lambda = 190 nm and the optical band gap is estimated to be 6.52 eV, which is in good agreement with the experimental data (6.526 eV). The energy gap value confirms that Li3B5O8(OH)(2) exhibits an exceptional laser damage threshold and is expected to produce coherent radiation in the deep-ultraviolet (DUV) region. The obtained value of SHG at lambda = 1064 nm is about 1.5 times that of the well-known NLO crystal KH2PO4 (KDP) at lambda = 1064 nm and 3.5 times that of KDP at lambda = 190 nm, which is transparent down to the DUV region. Thus, one can conclude that the combination of an alkali metal with borates leads to the generation of promising DUV-NLO crystals. This work is aimed at qualitative and quantitative investigation to report a reliable SHG value and provide details of the NLO tensor for bulk Li3B5O8(OH)(2) single crystals.

Accession Number: WOS:000416054400041

PubMed ID: 29120475

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363

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Record 11 of 491

Title: Competing phases in a model of Pr-based cobaltites

Author(s): Sotnikov, A (Sotnikov, A.); Kunes, J (Kunes, J.)

Source: PHYSICAL REVIEW B **Volume:** 96 **Issue:** 24 **Article Number:** 245102 **DOI:** 10.1103/PhysRevB.96.245102 **Published:** DEC 4 2017

Abstract: Motivated by the physics of Pr-based cobaltites, we study the effect of the external magnetic field in the hole-doped two-band Hubbard model close to instabilities toward the excitonic condensation and ferromagnetic ordering. Using the dynamical mean-field theory we observe a field-driven suppression of the excitonic condensate. The onset of a magnetically ordered phase at the fixed chemical potential is accompanied by a sizable change of the electron density. This leads us to predict that Pr3+ abundance increases on the high-field side of the transition.

Accession Number: WOS:000416943900002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sotnikov, Andrii	A-7274-2015	0000-0002-3632-4790
Kunes, Jan	B-4484-2008	0000-0001-9682-7640

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Record 12 of 491

Title: TIME-DEPENDENT NUMERICAL MODELING OF LARGE-SCALE ASTROPHYSICAL PROCESSES: FROM RELATIVELY SMOOTH FLOWS TO EXPLOSIVE EVENTS WITH EXTREMELY LARGE DISCONTINUITIES AND HIGH MACH NUMBERS

Author(s): Kurfurst, P (Kurfurst, Petr); Krticka, J (Krticka, Jiri)

Source: APPLICATIONS OF MATHEMATICS **Volume:** 62 **Issue:** 6 **Pages:** 633-659 **DOI:** 10.21136/AM.2017.0135-17 **Published:** DEC 2017

Abstract: We calculate self-consistent time-dependent models of astrophysical processes. We have developed two types of our own (magneto) hydrodynamic codes, either the operator-split, finite volume Eulerian code on a staggered grid for smooth hydrodynamic flows, or the finite volume unsplit code based on the Roe's method for explosive events with extremely large discontinuities and highly supersonic outbursts. Both the types of the codes use the second order Navier-Stokes viscosity to realistically model the viscous and dissipative effects. They are transformed to all basic orthogonal curvilinear coordinate systems as well as to a special non-orthogonal geometric system that fits to modeling of astrophysical disks. We describe mathematical background of our codes and their implementation for astrophysical simulations, including choice of initial and boundary conditions. We demonstrate some calculated models and compare the practical usage of numerically different types of codes.

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ISSN: 0862-7940

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Record 13 of 491

Title: Potential-Driven On/Off Switch Strategy for the Electrosynthesis of [7]Helicene-Derived Polymers

Author(s): Hrbac, J (Hrbac, Jan); Strasak, T (Strasak, Tomas); Fekete, L (Fekete, Ladislav); Ladanyi, V (Ladanyi, Vit); Pokorny, J (Pokorny, Jan); Bulir, J (Bulir, Jiri); Krbal, M (Krbal, Milos); Zadny, J (Zadny, Jaroslav); Storch, J (Storch, Jan); Vacek, J (Vacek, Jan)

Source: CHEMELECTROCHEM **Volume:** 4 **Issue:** 12 **Pages:** 3047-3052 **DOI:** 10.1002/celc.201700441 **Published:** DEC 2017

Abstract: New materials bearing thiophene and helicene moieties were prepared by using a potential-driven on/off switch strategy on the surface of glassy carbon and indium tin oxide substrates. Specifically, a 3-([7] helicen-9-yl)-thiophene hybrid monomer was electrooxidized in acetonitrile by using cyclic voltammetry with anodic potential limits of + 1.5 or + 2.5 V, resulting in a conductive and non-conductive polymer, respectively. The electrochemical findings were supplemented by microscopy investigations, UV/Vis, fluorescence and vibrational spectroscopies, and H-1 NMR spectroscopy as well as ellipsometry measurements and computational chemistry. The electrodeposited polymers could be used for the further development of materials applicable in organic electronics, optoelectronics, and sensing technologies.

Accession Number: WOS:000419269000004

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zadny, Jaroslav		0000-0002-3737-3519

ISSN: 2196-0216

Record 14 of 491

Title: Vapor Pressures and Thermophysical Properties of Ethylene Carbonate, Propylene Carbonate, gamma-Valerolactone, and gamma-Butyrolactone

Author(s): Pokorny, V (Pokorny, Vaclav); Stejfa, V (Stejfa, Vojtech); Fulem, M (Fulem, Michal); Cervinka, C (Cervinka, Ctirad); Ruzicka, K (Ruzicka, Kvetoslav)

Source: JOURNAL OF CHEMICAL AND ENGINEERING DATA **Volume:** 62 **Issue:** 12 **Pages:** 4174-4186 **DOI:** 10.1021/acs.jced.7b00578 **Published:** DEC 2017

Abstract: In this work, a thermodynamic study of four important industrial solvents, ethylene carbonate (CAS RN: 96-49-1), propylene carbonate (CAS RN: 108-32-7), gamma-valerolactone (CAS RN: 108-29-2), and gamma-butyrolactone (CAS RN: 96-48-0), is presented. The vapor pressure measurements were performed by static method using two apparatuses in a combined temperature interval (238-363) K. Heat capacities of condensed phases were measured by Tian-Calvet calorimetry in the temperature interval (262-358) K. The phase behavior of ethylene carbonate and gamma-valerolactone was investigated by a heat-flux DSC from 183-303 and 328 K, respectively. Ideal-gas thermodynamic properties were calculated using the methods of statistical thermodynamics based on calculated fundamental vibrational frequencies and molecular structure data. A consistent thermodynamic description of all involved properties (calculated ideal-gas heat capacities and experimental data on vapor pressures, condensed phase heat capacities, and vaporization enthalpies) was achieved by their simultaneous correlation.

Accession Number: WOS:000418393800014

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ruzicka, Kvetoslav	B-1071-2008	0000-0001-9048-1036
Pokorny, Vaclav		0000-0003-4145-7982

ISSN: 0021-9568

Record 15 of 491

Title: Kinetics of the Raman scattering in a laser corona using a transform method

Author(s): Masek, M (Masek, M.); Rohlena, K (Rohlena, K.)

Source: LASER AND PARTICLE BEAMS **Volume:** 35 **Issue:** 4 **Pages:** 687-698 **DOI:** 10.1017/S0263034617000696 **Published:** DEC 2017

Abstract: This paper is an extension of our previous paper (Maek and Rohlena, 2015), where we applied a transform method for the solution of Vlasov-Maxwell set of equations in a one-dimensional geometry to describe the Raman backscattering of the heating ns laser wave in the external corona of the generated laser plasma in a strongly non-linear regime. The method is stabilized by a simplified Fokker-Planck collision term, which, in turn, is used for a study of the influence of collisional and collisionless damping mechanisms of the daughter electron plasma wave (EPW) on the instability development and their competition resulting in a different instability behavior in various plasma configurations. The physics of trapped electrons is studied in detail and compared to the resulting Raman reflectivity. The Raman reflectivity was found to depend strongly on the intensity of laser irradiation in the different regions of the plasma corona. This is discussed in detail from the point of view of trapped electrons behavior in the EPW. Moreover, a study of the Raman reflectivity dependence on the electron-ion collision frequency (average plasma ionization) is presented, too. The results supplement the physical picture of the collision and collisionless processes influencing the Raman instability non-linear development.

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Record 16 of 491

Title: Formation of Staphylococcus aureus Biofilm in the Presence of Sublethal Concentrations of Disinfectants Studied via a Transcriptomic Analysis Using Transcriptome Sequencing (RNA-seq)

Author(s): Slany, M (Slany, M.); Oppelt, J (Oppelt, J.); Cincarova, L (Cincarova, L.)

Source: APPLIED AND ENVIRONMENTAL MICROBIOLOGY **Volume:** 83 **Issue:** 24 **Article Number:** UNSP e01643-17 **DOI:** 10.1128/AEM.01643-17 **Published:** DEC 2017

Abstract: Staphylococcus aureus is a common biofilm-forming pathogen. Low doses of disinfectants have previously been reported to promote biofilm formation and to increase virulence. The aim of this study was to use transcriptome sequencing (RNA-seq) analysis to investigate global transcriptional changes in S. aureus in response to sublethal concentrations of the commonly used food industry disinfectants ethanol (EtOH) and chloramine T (ChT) and their combination (EtOH_ChT) in order to better understand the effects of these agents on biofilm formation. Treatment with EtOH and EtOH_ChT resulted in more significantly altered expression profiles than treatment with ChT. Our results revealed that EtOH and EtOH_ChT treatments enhanced the expression of genes responsible for regulation of gene expression (sigB), cell surface factors (clfAB), adhesins (sdrDE), and capsular polysaccharides (cap8EFGL), resulting in more intact biofilm. In addition, in this study we were able to identify the pathways involved in the adaptation of S. aureus to the stress of ChT treatment. Further, EtOH suppressed the effect of ChT on gene expression when these agents were used together at sublethal concentrations. These data show that in the presence of sublethal concentrations of tested disinfectants, S. aureus cells trigger protective mechanisms and try to cope with them.
IMPORTANCE So far, the effect of disinfectants is not satisfactorily explained. The presented data will allow a better understanding of the mode of disinfectant action with regard to biofilm formation and the ability of bacteria to survive the treatment. Such an understanding could contribute to the effort to eliminate possible sources of bacteria, making disinfectant application as efficient as possible. Biofilm formation plays significant role in the spread and pathogenesis of bacterial species.

Accession Number: WOS:000416937000008

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Oppelt, Jan	H-7388-2017	0000-0002-3076-4840

ISSN: 0099-2240

eISSN: 1098-5336

Record 17 of 491

Title: GLASS: assisted and standardized assessment of gene variations from Sanger sequence trace data

Author(s): Pal, K (Pal, Karol); Bystry, V (Bystry, Vojtech); Reigl, T (Reigl, Tomas); Demko, M (Demko, Martin); Krejci, A (Krejci, Adam); Touloumenidou, T (Touloumenidou, Tasoula); Stalika, E (Stalika, Evangelia); Tichy, B (Tichy, Boris); Ghia, P (Ghia, Paolo); Stamatopoulos, K (Stamatopoulos, Kostas); Pospisilova, S (Pospisilova, Sarka); Malcikova, J (Malcikova, Jitka); Darzentas, N (Darzentas, Nikos)

Group Author(s): European Res Initiative CLL ERIC-T

Source: BIOINFORMATICS **Volume:** 33 **Issue:** 23 **Pages:** 3802-3804 **DOI:** 10.1093/bioinformatics/btx423 **Published:** DEC 1 2017

Abstract: Motivation: Sanger sequencing is still being employed for sequence variant detection by many laboratories, especially in a clinical setting. However, chromatogram interpretation often requires manual inspection and in some cases, considerable expertise.
Results: We present GLASS, a web-based Sanger sequence trace viewer, editor, aligner and variant caller, built to assist with the assessment of variations in 'curated' or user-provided genes. Critically, it produces a standardized variant output as recommended by the Human Genome Variation Society.
Accession Number: WOS:000417004100017
PubMed ID: 29036643
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Tichy, Boris	C-1314-2009	0000-0001-9252-7974

ISSN: 1367-4803
eISSN: 1460-2059

Record 18 of 491

Title: Interaction of lysozyme with a tear film lipid layer model: A molecular dynamics simulation study
Author(s): Wizert, A (Wizert, Alicia); Iskander, DR (Iskander, D. Robert); Cwiklik, L (Cwiklik, Lukasz)
Source: BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES **Volume:** 1859 **Issue:** 12 **Pages:** 2289-2296 **DOI:** 10.1016/j.bbamem.2017.08.015 **Published:** DEC 2017
Abstract: The tear film is a thin multilayered structure covering the cornea. Its outermost layer is a lipid film underneath of which resides on an aqueous layer. This tear film lipid layer (TFLL) is itself a complex structure, formed by both polar and nonpolar lipids. It was recently suggested that due to tear film dynamics, TFLL contains in homogeneities in the form of polar lipid aggregates. The aqueous phase of tear film contains lachrymal-origin proteins, whereby lysozyme is the most abundant. These proteins can alter TFLL properties, mainly by reducing its surface tension. However, a detailed nature of protein-lipid interactions in tear film is not known. We investigate the interactions of lysozyme with TFLL in molecular details by employing coarse-grained molecular dynamics simulations. We demonstrate that lysozyme, due to lateral restructuring of TFLL, is able to penetrate the tear lipid film embedded in inverse micellar aggregates.
Accession Number: WOS:000415770900002
PubMed ID: 28847503
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cwiklik, Lukasz	A-7206-2008	0000-0002-2083-8738

ISSN: 0005-2736
eISSN: 0006-3002

Record 19 of 491

Title: Lone pair-pi interactions in biological systems: occurrence, function, and physical origin
Author(s): Kozelka, J (Kozelka, Jiri)
Source: EUROPEAN BIOPHYSICS JOURNAL WITH BIOPHYSICS LETTERS **Volume:** 46 **Issue:** 8 **Special Issue:** SI **Pages:** 729-737 **DOI:** 10.1007/s00249-017-1210-1 **Published:** DEC 2017
Abstract: Lone pair-pi interactions are now recognized as a supramolecular bond whose existence in biological systems is documented by a growing number of examples. They are commonly attributed to electrostatic forces. This review attempts to highlight some recent discoveries evidencing the important role which lone pair-pi interactions, and anion-pi interactions in particular, play in stabilizing the structure and affecting the function of biomolecules. Special attention is paid to studies exploring the physical origin of these at first glance counterintuitive interactions between a lone pair of electrons of one residue and the pi-cloud of another. Recent theoretical work went beyond the popular electrostatic model and inquired the extent to which orbital interactions have to be taken into account. In at least one biologically relevant case-that of anion-flavin interactions-a substantial charge-transfer component has been shown to operate.
Accession Number: WOS:000415817400005
PubMed ID: 28466098
Conference Title: 7th Regional Biophysics Conference (RBC)
Conference Date: AUG 25-28, 2016
Conference Location: Univ Trieste, Trieste, ITALY
Conference Sponsors: Italian Soc Pure & Appl Biophys, CNR Inst Biophys, Univ Trieste, Dept Life Sci
Conference Host: Univ Trieste
ISSN: 0175-7571
eISSN: 1432-1017

Record 20 of 491

Title: Segregation of sp-impurities at grain boundaries and surfaces: comparison of fcc cobalt and nickel
Author(s): Vsianska, M (Vsianska, M.); Vemolova, H (Vemolova, H.); Sob, M (Sob, M.)
Source: MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING **Volume:** 25 **Issue:** 8 **Article Number:** 085004 **DOI:** 10.1088/1361-651X/aa86bf **Published:** DEC 2017
Abstract: We perform systematic ab initio investigations of the segregation of 12 nonmagnetic sp-impurities (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) at the Sigma 5 (210) grain boundary (GB) and (210) free surface (FS) in fcc ferromagnetic cobalt and analyse their effect on structural, magnetic and mechanical properties; the results are compared with those obtained previously for nickel. It turns out that there is a slight enhancement of magnetization at the clean GB and FS with respect to bulk cobalt (4.7% and 17%, respectively). However, segregated sp-impurities sharply reduce this magnetization. As shown previously, in nickel most of the above impurities nearly destroy or substantially reduce the magnetic moments at the FS and, when segregated interstitially (i.e. Si, P, S, Ge, As, and Se), also at the GB, so that they provide atomically thin, magnetically dead layers, which may be very desirable in spintronics. The reduction of magnetic moments at the Sigma 5(210) GB in fcc ferromagnetic cobalt is, in absolute values, very similar to that in nickel. However, as the magnetic moment in bulk cobalt is higher, we do not observe magnetically dead layers here. Further, we find the preferred segregation sites at the Sigma 5(210) GB for the sp-impurities studied, and their segregation enthalpies and strengthening/embrittling energies with their decomposition into their chemical and mechanical components. It turns out that interstitially segregated Si is a GB cohesion enhancer, and interstitially segregated P, S, Ge, As, and Se and substitutionally segregated Al, Ga, In, Sn, Sb and Te are GB embrittlers in fcc cobalt. As there is essentially no experimental information on GB segregation in cobalt, most of the present results are theoretical predictions which may motivate future experimental work.
Accession Number: WOS:000413837100001
ISSN: 0965-0393
eISSN: 1361-651X

Record 21 of 491

Title: Electromagnetic characteristics of geodesic acoustic mode in the COMPASS tokamak
Author(s): Seidl, J (Seidl, J.); Krbec, J (Krbec, J.); Hron, M (Hron, M.); Adamek, J (Adamek, J.); Hidalgo, C (Hidalgo, C.); Markovic, T (Markovic, T.); Melnikov, AV (Melnikov, A. V.); Stockel, J (Stockel, J.); Weinzettl, V (Weinzettl, V.); Aftanas, M (Aftanas, M.); Bilkova, P (Bilkova, P.); Bogar, O (Bogar, O.); Bohm, P (Bohm, P.); Eliseev, LG (Eliseev, L. G.); Hacek, P (Hacek, P.); Havlicek, J (Havlicek, J.); Horacek, J (Horacek, J.); Imrisek, M (Imrisek, M.); Kovarik, K (Kovarik, K.); Mitosinkova, K (Mitosinkova, K.); Panek, R (Panek, R.); Tomes, M (Tomes, M.); Vondracek, P (Vondracek, P.)
Source: NUCLEAR FUSION **Volume:** 57 **Issue:** 12 **Article Number:** 126048 **DOI:** 10.1088/1741-4326/aa897e **Published:** DEC 2017
Abstract: Axisymmetric geodesic acoustic mode (GAM) oscillations of the magnetic field, plasma potential and electron temperature have been identified on the COMPASS tokamak. This work brings an overview of their electromagnetic properties studied by multi-pin reciprocating probes and magnetic diagnostics. The n = 0 fluctuations form a continuous spectrum in limited plasmas but change to a single dominant peak in diverted configuration. At the edge of diverted plasmas the mode exhibits a non-local structure with a constant frequency over a radial extent of at least several centimeters. Nevertheless, the frequency still reacts on temporal changes of plasma temperature caused by an auxiliary NBI heating as well as those induced by periodic sawtooth crashes. Radial wavelength of the mode is found to be about 1-4 cm, with values larger for the plasma potential than for the electron temperature. The mode propagates radially outward and its radial structure induces oscillations of a poloidal E x B velocity, that can locally reach the level of the mean poloidal flow. Bicoherence analysis confirms a non-linear interaction of GAM with a broadband ambient turbulence. The mode exhibits strong axisymmetric magnetic oscillations

that are studied both in the poloidal and radial components of the magnetic field. Their poloidal standing-wave structure was confirmed and described for the first time in diverted plasmas. In limited plasmas their amplitude scales with safety factor. Strong suppression of the magnetic GAM component, and possibly of GAM itself, is observed during co-current but not counter-current NBI.

Accession Number: WOS:000413136900002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Havlicek, Josef	G-2897-2014	0000-0002-7047-5007
Kovarik, Karel	G-3496-2014	0000-0002-1049-0504
Bilkova, Petra	G-9496-2014	
Horacek, Jan	G-8301-2014	0000-0002-4276-3124
Adamek, Jiri	G-7421-2014	
Weinzettl, Vladimir	G-3657-2014	0000-0001-8936-7578
Seidl, Jakub	G-3413-2014	
Vondracek, Petr	G-6786-2014	0000-0003-0125-9252
Krbec, Jaroslav		0000-0002-3780-6257

ISSN: 0029-5515

eISSN: 1741-4326

Record 22 of 491

Title: Ab initio thermodynamic properties and their uncertainties for crystalline alpha-methanol

Author(s): Cervinka, C (Cervinka, Ctirad); Beran, GJO (Beran, Gregory J. O.)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 44 **Pages:** 29940-29953 **DOI:** 10.1039/c7cp06605h **Published:** NOV 28 2017

Abstract: To investigate the performance of quasi-harmonic electronic structure methods for modeling molecular crystals at finite temperatures and pressures, thermodynamic properties are calculated for the low-temperature alpha polymorph of crystalline methanol. Both density functional theory (DFT) and ab initio wavefunction techniques up to coupled cluster theory with singles, doubles, and perturbative triples (CCSD(T)) are combined with the quasi-harmonic approximation to predict energies, structures, and properties. The accuracy, reliability, and uncertainties of the individual quantum-chemical methods are assessed via detailed comparison of calculated and experimental data on structural properties (density) and thermodynamic properties (isobaric heat capacity). Performance of individual methods is also studied in context of the hierarchy of the quantum-chemical methods. The results indicate that while some properties such as the sublimation enthalpy and thermal expansivity can be modeled fairly well, other properties such as the molar volume and isobaric heat capacities are harder to predict reliably. The errors among the energies, structures, and phonons are closely coupled, and most accurate predictions here appear to arise from fortuitous error compensation among the different contributions. This study highlights how sensitive molecular crystal property predictions can be to the underlying model approximations and the significant challenges inherent in first-principles predictions of solid state structures and thermochemistry.

Accession Number: WOS:000415576800025

PubMed ID: 29090305

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Beran, Gregory	B-8684-2011	0000-0002-2229-2580

ISSN: 1463-9076

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Record 23 of 491

Title: Free-Energy Surface Prediction by Flying Gaussian Method: Multisystem Representation

Author(s): Kriz, P (Kriz, Pavel); Sucur, Z (Sucur, Zoran); Spiwok, V (Spiwok, Vojtech)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 121 **Issue:** 46 **Pages:** 10479-10483 **DOI:** 10.1021/acs.jpcb.7b09337 **Published:** NOV 23 2017

Abstract: Flying Gaussian method simulates multiple replicas of the studied system and enhances sampling by disfavoring replicas to simultaneously sample similar states. The bias potential used for this enhancement is highly dynamic when looking at individual replica, which raises concerns about the accuracy of free-energy surfaces predicted by reweighing methods. Here we show that the bias potential can be considered as static when looking at the simulation from a multisystem perspective. We present two equations that can be used to predict the free-energy surface, and we demonstrate their convergence.

Accession Number: WOS:000416495800006

PubMed ID: 29072909

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Spiwok, Vojtech	A-7747-2008	0000-0001-8108-2033

ISSN: 1520-6106

Record 24 of 491

Title: 2D Material Armors Showing Superior Impact Strength of Few Layers

Author(s): Signetti, S (Signetti, Stefano); Taioli, S (Taioli, Simone); Pugno, NM (Pugno, Nicola M.)

Source: ACS APPLIED MATERIALS & INTERFACES **Volume:** 9 **Issue:** 46 **Pages:** 40820-40830 **DOI:** 10.1021/acsami.7b12030 **Published:** NOV 22 2017

Abstract: We study the ballistic properties of two-dimensional (2D) materials upon the hypervelocity impacts of C-60 fullerene molecules combining ab initio density functional tight binding and finite element simulations. The critical penetration energy of monolayer membranes is determined using graphene and the 2D allotrope of boron nitride as case studies. Furthermore, the energy absorption scaling laws with a variable number of layers and interlayer spacing are investigated, for homogeneous or hybrid configurations (alternated stacking of graphene and boron nitride). At the nanolevel, a synergistic interaction between the layers emerges, not observed at the micro- and macro-scale for graphene armors. This size-scale transition in the impact behavior toward higher dimensional scales is rationalized in terms of scaling of the damaged volume and material strength. An optimal number of layers, between 5 and 10, emerges demonstrating that few-layered 2D material armors possess impact strength even higher than their monolayer counterparts. These results provide fundamental understanding for the design of ultralightweight multilayer armors using enhanced 2D material-based nanocomposites.

Accession Number: WOS:000416614600105

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Taioli, Simone		0000-0003-4010-8000

ISSN: 1944-8244

Record 25 of 491

Title: First-principles-based Landau-Devonshire potential for BiFeO3

Author(s): Marton, P (Marton, P.); Klic, A (Klic, A.); Pasciak, M (Pasciak, M.); Hlinka, J (Hlinka, J.)

Source: PHYSICAL REVIEW B **Volume:** 96 **Issue:** 17 **Article Number:** 174110 **DOI:** 10.1103/PhysRevB.96.174110 **Published:** NOV 17 2017

Abstract: The work describes a first-principles-based computational strategy for studying structural phase transitions, and in particular, for determination of the so-called Landau-Devonshire potential-the classical zero-temperature limit of the Gibbs energy, expanded in terms of order parameters. It exploits the configuration space attached to the eigenvectors of the modes frozen in the ground state, rather than the space spanned by the unstable modes of the high-symmetry phase, as done usually. This allows us to carefully probe the part of the energy surface in the vicinity of the ground state, which is most relevant for the properties of the ordered phase. We apply this procedure to BiFeO3 and perform ab initio calculations in order to determine potential energy contributions associated with strain, polarization, and oxygen octahedra tilt degrees of freedom, compatible with its two-formula unit cell periodic boundary conditions.

Accession Number: WOS:000415567500001

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Marton, Pavel	G-1611-2011	0000-0001-7273-7288
Pasciak, Marek		0000-0002-3902-8874

ISSN: 2469-9950
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Record 26 of 491

Title: Limitations in the description of conformational preferences of C-disaccharides: The (1 -> 3)-C-mannobiose case
Author(s): Raich, I (Raich, Ivan); Lovyova, Z (Lovyova, Zuzana); Trnka, L (Trnka, Ladislav); Parkan, K (Parkan, Kamil); Kessler, J (Kessler, Jiri); Pohl, R (Pohl, Radek); Kaminsky, J (Kaminsky, Jakub)
Source: CARBOHYDRATE RESEARCH **Volume:** 451 **Pages:** 42-50 **DOI:** 10.1016/j.carres.2017.09.006 **Published:** NOV 8 2017
Abstract: Conformational preferences of two C-glycosyl analogues of Manp-(1 -> 3)-Manp, were studied using a combined method of theoretical and experimental chemistry. Molecular dynamics was utilized to provide conformational behavior along C-glycosidic bonds of methyl 3-deoxy-3-C-[(alpha-D-mannopyranosyl) methyl]-alpha-D-and L-mannopyranosides. The OPLS2005 and Glycam06 force fields were used. Simulations were performed with explicit water (TIP3P) and methanol. Results were compared with a complete conformational scan at the MM4 level with the dielectric constant corresponding to methanol. In order to verify predicted conformational preferences, vicinal (3)J(HH) NMR coupling constants were calculated by the Karplus equation on simulated potential energy surfaces (PES). A set of new parameters for the Karplus equation was also designed. Predicted 3JHH were compared with experimental data. We also used reverse methodology, in which the (3)J(HH) coupling constants were calculated at the DFT level for each family of (phi, psi)-conformers separately and then experimental values were decomposed onto calculated (3)J(HH) couplings in order to obtain experimentally derived populations of conformers. As an alternative method of evaluation of preferred conformers, analysis of sensitive C-13 chemical shifts was introduced. We were able to thoroughly discuss several fundamental issues in predictions of preferred conformers of C-saccharides, such as the solvent effect, reliability of the force field, character of empirical Karplus equation or applicability of NMR parameters in predictions of conformational preferences in general. (C) 2017 Elsevier Ltd. All rights reserved.
Accession Number: WOS:000413320300005
PubMed ID: 28950209
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022
Parkan, Kamil	F-1138-2017	0000-0001-7585-6004
Raich, Ivan		0000-0002-1603-0445

ISSN: 0008-6215
eISSN: 1873-426X

Record 27 of 491

Title: Self-assembled clusters of patchy rod-like molecules
Author(s): Jurasek, M (Jurasek, Miroslav); Vacha, R (Vacha, Robert)
Source: SOFT MATTER **Volume:** 13 **Issue:** 41 **Pages:** 7492-7497 **DOI:** 10.1039/c7sm01384a **Published:** NOV 4 2017
Abstract: The design of complex self-assembled structures remains a challenging task due to the intricate relationship between the properties of the building blocks and the final morphology of the aggregates. Here, we report such a relationship for rod-like particles with one or two attractive patches based on a combination of computer simulations and analytical theory. We investigated the formation of finite aggregates under various conditions and constructed structure diagrams, which can be used to determine and extrapolate the system composition. The size of the clusters is mainly determined by the size of the attractive patches and their geometrical arrangement. We showed that it is challenging to obtain clusters with more than four particles in high yields, and more complex building blocks or additional molecules would need to be used. Moreover, the particles with patch sizes close to the structure boundaries can switch between the aggregate state by a small change in conditions. These findings can be useful for the development of self-assembling building blocks and for the understanding of protein folds of coiled coils under various conditions.
Accession Number: WOS:000413794700004
PubMed ID: 28932858
ISSN: 1744-683X
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Record 28 of 491

Title: Legionella Becoming a Mutualist: Adaptive Processes Shaping the Genome of Symbiont in the Louse Polyplax serrata
Author(s): Rihova, J (Rihova, Jana); Novakova, E (Novakova, Eva); Husnik, F (Husnik, Filip); Hypsa, V (Hypsa, Vaclav)
Source: GENOME BIOLOGY AND EVOLUTION **Volume:** 9 **Issue:** 11 **Pages:** 2946-2957 **DOI:** 10.1093/gbe/evx217 **Published:** NOV 2017
Abstract: Legionellaceae are intracellular bacteria known as important human pathogens. In the environment, they are mainly found in biofilms associated with amoebas. In contrast to the gammaproteobacterial family Enterobacteriaceae, which established a broad spectrum of symbioses with many insect taxa, the only instance of legionella-like symbiont has been reported from lice of the genus Polyplax. Here, we sequenced the complete genome of this symbiont and compared its main characteristics to other Legionella species and insect symbionts. Based on rigorous multigene phylogenetic analyses, we confirm this bacterium as a member of the genus Legionella and propose the name Candidatus Legionella polyplacis, sp. n. We show that the genome of Ca. Legionella polyplacis underwent massive degeneration, including considerable size reduction (529.746 bp, 484 protein coding genes) and a severe decrease in GC content (23%). We identify several possible constraints underlying the evolution of this bacterium. On one hand, Ca. Legionella polyplacis and the louse symbionts Riesia and Puchtella experienced convergent evolution, perhaps due to adaptation to similar hosts. On the other hand, somemetabolic differences are likely to reflect different phylogenetic positions of the symbionts and hence availability of particular metabolic function in the ancestor. This is exemplified by different arrangements of thiamine metabolism in Ca. Legionella polyplacis and Riesia. Finally, horizontal gene transfer is shown to play a significant role in the adaptive and diversification process. Particularly, we show that Ca. L. polyplacis horizontally acquired a complete biotin operon (bioADCHFB) that likely assisted this bacterium when becoming an obligate mutualist.
Accession Number: WOS:000423459700002
PubMed ID: 29069349
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Novakova, Eva	D-9475-2016	0000-0003-4090-0655
Husnik, Filip		0000-0002-5381-0125

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Record 29 of 491

Title: The MADLA planner: Multi-agent planning by combination of distributed and local heuristic search
Author(s): Stolba, M (Stolba, Michal); Komenda, A (Komenda, Antonin)
Source: ARTIFICIAL INTELLIGENCE **Volume:** 252 **Pages:** 175-210 **DOI:** 10.1016/j.artint.2017.08.007 **Published:** NOV 2017
Abstract: Real world applications often require cooperation of multiple independent entities. Classical planning is a well established technique solving various challenging problems such as logistic planning, factory process planning, military mission planning and high-level planning for robots. Multi-agent planning aims at solving similar problems in the presence of multiple independent entities (agents). Even though such entities might want to cooperate in order to fulfill a common goal, they may want to keep their internal information and processes private. In such case, we talk about privacy-preserving multi agent planning.
So far, multi-agent planners based on heuristic search used either a local heuristic estimating the particular agent's local subproblem or a distributed heuristic estimating the global problem as a whole. In this paper, we present the Multi-Agent Distributed and Local Asynchronous (MADLA) Planner, running a novel variant of a distributed state space forward-chaining multi-heuristic search which combines the use of a local and a distributed heuristic in order to combine their benefits. In particular, the planner uses two variants of the well known Fast-Forward heuristic. We provide proofs of soundness and completeness of the search algorithm and show how much and what type of privacy it preserves. We also provide an improved privacy-preserving distribution scheme for the Fast-Forward heuristic.
We experimentally compare the newly proposed multi-heuristic scheme and the two used heuristics separately. The results show that the proposed solution outperforms classical (single-heuristic) distributed search with either one of the heuristics used separately. In the detailed experimental analysis, we show limits of the planner and of the used heuristics based on particular properties of the benchmark domains. In a comprehensive set of multi agent planning domains and problems, we show that the MADLA Planner outperforms all

contemporary state-of-the-art privacy-preserving multi-agent planners using a compatible planning model. (C) 2017 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Komenda, Antonin		0000-0002-6947-308X

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Record 30 of 491

Title: Analysis of dermal fibroblasts isolated from neonatal and child cleft lip and adult skin: Developmental implications on reconstructive surgery

Author(s): Zivicova, V (Zivicova, Veronika); Lacina, L (Lacina, Lukas); Mateu, R (Mateu, Rosana); Smetana, K (Smetana, Karel, Jr.); Kavkova, R (Kavkova, Radana); Krejci, ED (Krejci, Eliska Drobna); Grim, M (Grim, Milos); Kvasilova, A (Kvasilova, Alena); Borsky, J (Borsky, Jiri); Strnad, H (Strnad, Hynek); Hradilova, M (Hradilova, Miluse); Sachova, J (Sachova, Jana); Kolar, M (Kolar, Michal); Dvorankova, B (Dvorankova, Barbora)

Source: INTERNATIONAL JOURNAL OF MOLECULAR MEDICINE **Volume:** 40 **Issue:** 5 **Pages:** 1323-1334 **DOI:** 10.3892/ijmm.2017.3128 **Published:** NOV 2017

Abstract: The nonsyndromic cleft is one of the most frequent congenital defects in humans. Clinical data demonstrated improved and almost scarless neonatal healing of reparative surgery. Based on our previous results on crosstalk between neonatal fibroblasts and adult keratinocytes, the present study focused on characterization of fibroblasts prepared from cleft lip tissue samples of neonates and older children, and compared them with samples isolated from normal adult skin (face and breast) and scars. Although subtle variances in expression profiles of children and neonates were observed, the two groups differed significantly from adult cells. Compared with adult cells, differences were observed in nestin and smooth muscle actin (SMA) expression at the protein and transcript level. Furthermore, fibroblast to myofibroblast differentiation drives effective wound healing and is largely regulated by the cytokine, transforming growth factor-beta 1 (TGF-beta 1). Dysregulation of the TGF-beta signalling pathway, including low expression of the TGF-beta receptor II, may contribute to reducing scarring in neonates. Fibroblasts of facial origin also exhibited age independent differences from the cells prepared from the breast, reflecting the origin of the facial cells from neural crest-based ectomesenchyme.

Accession Number: WOS:000413398800003

PubMed ID: 28901389

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Krejci, Eliska	G-3034-2014	0000-0002-3394-9971
Grim, Milos	H-6066-2017	0000-0001-5280-0091
Dvorankova, Barbora	R-2316-2016	0000-0002-3914-9668
Kolar, Michal	A-3307-2012	0000-0002-4593-1525
Kvasilova, Alena		0000-0002-2399-0428

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Record 31 of 491

Title: Force field parametrization of hydrogenoxalate and oxalate anions with scaled charges

Author(s): Kroutil, O (Kroutil, Ondrej); Predota, M (Predota, Milan); Kabelac, M (Kabelac, Martin)

Source: JOURNAL OF MOLECULAR MODELING **Volume:** 23 **Issue:** 11 **Article Number:** 327 **DOI:** 10.1007/s00894-017-3490-x **Published:** NOV 2017

Abstract: Models of the hydrogenoxalate (bioxalate, charge -1) and oxalate (charge -2) anions were developed for classical molecular dynamics (CMD) simulations and parametrized against ab initio molecular dynamics (AIMD) data from our previous study (Kroutil et al. (2016) J Mol Model 22: 210). The interactions of the anions with water were described using charges scaled according to the electronic continuum correction approach with rescaling of nonbonded parameters (ECCR), and those descriptions of anion interactions were found to agree well with relevant AIMD and experimental results. The models with full RESP charges showed excessively strong electrostatic interactions between the solute and water molecules, leading to an overstructured solvation shell around the anions and thus to a diffusion coefficient that was much too low. The effect of charge scaling was more evident for the oxalate dianion than for the hydrogenoxalate anion. Our work provides CMD models for ions of oxalic acid and extends previous studies that showed the importance of ECCR for modeling divalent ions and ions of organic compounds.

Accession Number: WOS:000414003100001

PubMed ID: 29080940

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Predota, Milan	A-2256-2009	0000-0003-3902-0992

ISSN: 1610-2940

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Record 32 of 491

Title: Comparison of Microbiomes between Red Poultry Mite Populations (Dermanyssus gallinae): Predominance of Bartonella-like Bacteria

Author(s): Hubert, J (Hubert, Jan); Erban, T (Erban, Tomas); Kopecky, J (Kopecky, Jan); Sopko, B (Sopko, Bruno); Nesvorna, M (Nesvorna, Marta); Lichovnikova, M (Lichovnikova, Martina); Schicht, S (Schicht, Sabine); Strube, C (Strube, Christina); Sparagano, O (Sparagano, Olivier)

Source: MICROBIAL ECOLOGY **Volume:** 74 **Issue:** 4 **Pages:** 947-960 **DOI:** 10.1007/s00248-017-0993-z **Published:** NOV 2017

Abstract: Blood feeding red poultry mites (RPM) serve as vectors of pathogenic bacteria and viruses among vertebrate hosts including wild birds, poultry hens, mammals, and humans. The microbiome of RPM has not yet been studied by high-throughput sequencing. RPM eggs, larvae, and engorged adult/nymph samples obtained in four poultry houses in Czechia were used for microbiome analyses by Illumina amplicon sequencing of the 16S ribosomal RNA (rRNA) gene V4 region. A laboratory RPM population was used as positive control for transcriptome analysis by pyrosequencing with identification of sequences originating from bacteria. The samples of engorged adult/nymph stages had 100-fold more copies of 16S rRNA gene copies than the samples of eggs and larvae. The microbiome composition showed differences among the four poultry houses and among observed developmental stadia. In the adults' microbiome 10 OTUs comprised 90 to 99% of all sequences. Bartonella-like bacteria covered between 30 and 70% of sequences in RPM microbiome and 25% bacterial sequences in transcriptome. The phylogenetic analyses of 16S rRNA gene sequences revealed two distinct groups of Bartonella-like bacteria forming sister groups: (i) symbionts of ants; (ii) Bartonella genus. Cardinium, Wolbachia, and Rickettsiella sp. were found in the microbiomes of all tested stadia, while Spiroplasma eriocheiris and Wolbachia were identified in the laboratory RPM transcriptome. The microbiomes from eggs, larvae, and engorged adults/nymphs differed. Bartonella-like symbionts were found in all stadia and sampling sites. Bartonella-like bacteria was the most diversified group within the RPM microbiome. The presence of identified putative pathogenic bacteria is relevant with respect to human and animal health issues while the identification of symbiontic bacteria can lead to new control methods targeting them to destabilize the arthropod host.

Accession Number: WOS:000413625100019

PubMed ID: 28534089

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Erban, Tomas	F-9615-2011	0000-0003-1730-779X
Hubert, Jan	K-5489-2012	0000-0003-0740-166X
Sparagano, Olivier		0000-0003-3141-310X

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Record 33 of 491

Title: Brightness Temperature of Radio Zebras and Wave Energy Densities in Their Sources

Author(s): Yasnov, LV (Yasnov, L. V.); Benacek, J (Benacek, J.); Karlicky, M (Karlicky, M.)

Source: SOLAR PHYSICS **Volume:** 292 **Issue:** 11 **Article Number:** 163 **DOI:** 10.1007/s11207-017-1174-4 **Published:** NOV 2017
Abstract: We estimated the brightness temperature of radio zebras (zebra pattern - ZP), considering that ZPs are generated in loops having an exponential density profile in their cross section. We took into account that when in a plasma there is a source emitting in all directions, then in the escape process from the plasma the emission has a directional character nearly perpendicular to the constant-density profile. Owing to the high directivity of the plasma emission (for emission at frequencies close to the plasma frequency), the region from which the emission escapes can be very small. We estimated the brightness temperature of three observed ZPs for two values of the density scale height (1 and 0.21 Mm) and two values of the loop width (1 and 2 arcsec). In all cases, high brightness temperatures were obtained. For the higher value of the density scale height, the brightness temperature was estimated to be 1.1 x 10(15) -1.3 x 10(17) K, and for the lower value, it was 4.7 x 10(13) - 5.6 x 10(15) K. These temperatures show that the observational probability of a burst with a ZP, which is generated in the transition region with a steep gradient of the plasma density, is significantly higher than for a burst generated in a region with smoother changes of the plasma density. We also computed the saturation energy density of the upper-hybrid waves (according to the double plasma resonance model, they are generated in the zebra source) using a 3D particle-in-cell model with a loss-cone type of distribution of hot electrons. We found that this saturated energy is proportional to the ratio of hot electron and background plasma densities. Thus, comparing the growth rate and collisional damping of the upper-hybrid waves, we estimated minimum densities of hot electrons as well as the minimum value of the saturation energy density of the upper-hybrid waves. Finally, we compared the computed energy density of the upper-hybrid waves with the energy density of the electromagnetic waves in the zebra source and thus estimated the efficiency of the wave transformation.
Accession Number: WOS:000413851500001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Yasnov, Leonid	L-8265-2013	0000-0001-7164-9382
Karlicky, Marian	G-9023-2014	

ISSN: 0038-0938
eISSN: 1573-093X

Record 34 of 491

Title: Anomaly-based annotation error detection in speech-synthesis corpora

Author(s): Matousek, J (Matousek, Jindrich); Tihelka, D (Tihelka, Daniel)

Source: COMPUTER SPEECH AND LANGUAGE **Volume:** 46 **Pages:** 1-35 **DOI:** 10.1016/j.csl.2017.04.007 **Published:** NOV 2017
Abstract: We investigate the problem of automatic detection of annotation errors in single-speaker read-speech corpora used for speech synthesis. For the purpose of annotation error detection, we adopt an anomaly detection framework in which correctly annotated words are considered as normal examples on which the detection methods are trained. Misannotated words are then taken as anomalous examples which do not conform to normal patterns of the trained detection models. We propose and evaluate several anomaly detection models Gaussian distribution based detectors, Grubbs' test based detector, and one-class support vector machine based detector. Word-level feature sets including basic features derived from forced alignment and various acoustic, spectral, phonetic, and positional features are examined to find an optimal set of features for each anomaly detector. The results with F1 score being almost 89% show that anomaly detection could help detecting annotation errors in read-speech corpora for speech synthesis. Furthermore, dimensionality reduction techniques are also examined to automatically reduce the number of features used to describe the annotated words. We show that the automatically reduced feature sets achieve statistically similar results as the hand-crafted feature sets. We also conducted additional experiments to investigate both robustness of the proposed anomaly detection framework with respect to particular data sets used for development and evaluation and the influence of the number of examples needed for anomaly detection. We show that a reasonably good detection performance could be reached with using significantly fewer examples during the detector development phase. We also propose a concept of a voting detector a combination of anomaly detectors in which each "single" detector "votes" on whether or not a testing word is annotated correctly, and the final decision is then made by aggregating the votes. Our results show that the voting detector has a potential to overcome each of the single anomaly detectors. Furthermore, we compare the proposed anomaly detection framework to a classification-based approach (which, unlike anomaly detection, needs to use anomalous examples during training) and we show that both approaches lead to statistically comparable results when all available anomalous examples are utilized during detector/classifier development. However, when a smaller number of anomalous examples are used, the proposed anomaly detection framework clearly outperforms the classification-based approach. A final listening test showed the effectiveness of the proposed anomaly-based annotation error detection for improving the quality of synthetic speech. (C) 2017 Elsevier Ltd. All rights reserved.
Accession Number: WOS:000407609600001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Matousek, Jindrich	C-2146-2011	0000-0002-7408-7730

ISSN: 0885-2308
eISSN: 1095-8363

Record 35 of 491

Title: Novel borate CsZn2B3O7 single crystal with large efficient second harmonic generation in deep-ultraviolet spectral range

Author(s): Reshak, AH (Reshak, A. H.)

Source: JOURNAL OF ALLOYS AND COMPOUNDS **Volume:** 722 **Pages:** 438-444 **DOI:** 10.1016/j.jallcom.2017.06.126 **Published:** OCT 25 2017
Abstract: The linear and nonlinear optical susceptibility dispersion of CsZn2B3O7 single crystal are comprehensively investigated for a bulk structure in form of single crystal taking into account the influence of the packing structural units. The calculation highlights that the BO3 structural units packing is the main source for the large birefringence in CsZn2B3O7 due to high anisotropic electron distribution, and, hence, it affects the macroscopic second harmonic generation (SHG) coefficients. The large SHG is due to hyperpolarizablity formed by ZnO4 tetrahedra and co-parallel BO3 triangle groups. The absorption edge of CsZn2B3O7 occurs at lambda =218 nm and the optical band gap is estimated to be 5.68 eV that is in good agreement with the experimental data (5.69 eV). Therefore, CsZn2B3O7 is expected to produce a coherent radiation in deep-ultraviolet (DUV) region with SHG of about 1.5 x KDP (1.5x0.39 p. m./V=0.585 p. m./V) that agrees with the measurements. This work is aimed at the report of reliable SHG value and the details of the NLO tensor for bulk CsZn2B3O7 single crystal. (C) 2017 Elsevier B.V. All rights reserved.
Accession Number: WOS:000405520400058
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363

ISSN: 0925-8388
eISSN: 1873-4669

Record 36 of 491

Title: Adsorption and Diffusion of C-1 to C-4 Alkanes in Dual-Porosity Zeolites by Molecular Simulations

Author(s): Rezlerova, E (Rezlerova, Eliska); Zukal, A (Zukal, Arnost); Cejka, J (Cejka, Jiri); Siperstein, FR (Siperstein, Flor R.); Brennan, JK (Brennan, John K.); Lisal, M (Lisal, Martin)

Source: LANGMUIR **Volume:** 33 **Issue:** 42 **Pages:** 11126-11137 **DOI:** 10.1021/acs.langmuir.7b01772 **Published:** OCT 24 2017
Abstract: We employ grand canonical Monte Carlo and molecular dynamics simulations to systematically study the adsorption and diffusion of C-1 to C-4 alkanes in hierarchical ZSM-5 zeolite with micropores (similar to 1 nm) and mesopores (>2 nm). The zeolite is characterized by a large surface area of active sites on the microporous scale with high permeability and access to the active sites, which arises from the enhanced transport at the mesoporous scale. We model this zeolite as a microporous Na+-exchanged alumino-sillicate zeolite ZSM-S/35 (Si/Al = 3S) in which cylindrical mesopores with a diameter of 4 nm have been built by deleting atoms accordingly. We use the TraPPE and Vujic-Lyubartsev force fields along with the Lorentz-Berthelot combining rules to describe adsorbate adsorbate and adsorbate adsorbent interactions. The performance of the force fields is assessed by comparing against experimental single-component adsorption isotherms of methane and ethane in microporous ZSM-5/35, which we measured as part of this work. We compare the adsorption isotherms and diffusivities of the adsorbed alkanes in the dual-porosity zeolite with those in microporous ZSM-5/35 and discern the specific behavior at each porosity scale on the overall adsorption, self-diffusion, and transport behavior in zeolites with dual micro/mesoporosities.
Accession Number: WOS:000413992700005
PubMed ID: 28689411
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cejka, Jiri	B-1833-2013	0000-0003-1400-1031
Lisal, Martin	A-8176-2011	0000-0001-8005-7143
Siperstein, Flor		0000-0003-3464-2100

ISSN: 0743-7463

Record 37 of 491

Title: Eccentricity excitation and merging of planetary embryos heated by pebble accretion

Author(s): Chrenko, O (Chrenko, O.); Broz, M (Broz, M.); Lambrechts, M (Lambrechts, M.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 606 **Article Number:** A114 **DOI:** 10.1051/0004-6361/201731033 **Published:** OCT 23 2017

Abstract: Context. Planetary embryos can continue to grow by pebble accretion until they become giant planet cores. Simultaneously, these embryos mutually interact and also migrate due to torques arising from the protoplanetary disk.
Aims. Our aim is to study how pebble accretion alters the orbital evolution of embryos undergoing Type-I migration. In particular, we try to determine whether or not the embryos establish resonant chains, and if so, whether or not these chains are prone to instabilities. Further, we investigate the possibility that giant planet cores form through embryo merging which can be more rapid than pebble accretion alone.
Methods. For the first time, we perform self-consistent global-scale radiative hydrodynamic simulations of a two-fluid protoplanetary disk consisting of gas and pebbles, the latter being accreted by embedded embryos. Accretion heating, along with other radiative processes, is accounted for to correctly model the Type-I migration.
Results. We track the evolution of four super-Earth-like embryos, initially located in a region where the disk structure allows for a convergent migration. Generally, embryo merging is facilitated by rapidly increasing embryo masses and breaks the otherwise oligarchic growth. Moreover, we find that the orbital eccentricity of each embryo is considerably excited (similar or equal to 0.03) due to the presence of an asymmetric under-dense lobe of gas -a so-called "hot trail" -produced by accretion heating of the embryo's vicinity. Eccentric orbits lead the embryos to frequent close encounters and make resonant locking more difficult.
Conclusions. Embryo merging typically produces one massive core (greater than or similar to 10 M-E) in our simulations, orbiting near 10AU. Pebble accretion is naturally accompanied by the occurrence of eccentric orbits which should be considered in future efforts to explain the structure of exoplanetary systems.

Accession Number: WOS:000413564000003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Chrenko, Ondrej		0000-0001-7215-5026

ISSN: 1432-0746

Record 38 of 491

Title: Submolecular Resolution by Variation of the Inelastic Electron Tunneling Spectroscopy Amplitude and its Relation to the AFM/STM Signal

Author(s): de la Torre, B (de la Torre, Bruno); Svec, M (Svec, Martin); Foti, G (Foti, Giuseppe); Krejci, O (Krejci, Ondej); Hapala, P (Hapala, Prokop); Garcia-Lekue, A (Garcia-Lekue, Aran); Frederiksen, T (Frederiksen, Thomas); Zboril, R (Zboril, Radek); Arnau, A (Arnau, Andres); Vazquez, H (Vazquez, Hector); Jelinek, P (Jelinek, Pavel)

Source: PHYSICAL REVIEW LETTERS **Volume:** 119 **Issue:** 16 **Article Number:** 166001 **DOI:** 10.1103/PhysRevLett.119.166001 **Published:** OCT 16 2017

Abstract: Here we show scanning tunneling microscopy (STM), noncontact atomic force microscopy (AFM), and inelastic electron tunneling spectroscopy (IETS) measurements on an organic molecule with a CO-terminated tip at 5 K. The high-resolution contrast observed simultaneously in all channels unambiguously demonstrates the common imaging mechanism in STM/AFM/IETS, related to the lateral bending of the CO-functionalized tip. The IETS spectroscopy reveals that the submolecular contrast at 5 K consists of both renormalization of vibrational frequency and variation of the amplitude of the IETS signal. This finding is also corroborated by first principles simulations. We extend accordingly the probe-particle AFM/STM/IETS model to include these two main ingredients necessary to reproduce the high-resolution IETS contrast. We also employ the first principles simulations to get more insight into a different response of frustrated translation and rotational modes of the CO tip during imaging.

Accession Number: WOS:000413053700005

PubMed ID: 29099201

Author Identifiers:

Author	ResearcherID Number	ORCID Number
DONOSTIA INTERNATIONAL PHYSICS CTR., DIPC	C-3171-2014	
Krejci, Ondrej	G-5918-2014	0000-0002-4948-4312
Svec, Martin	G-6645-2014	
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922
Frederiksen, Thomas	D-3545-2011	0000-0001-7523-7641

ISSN: 0031-9007

eISSN: 1079-7114

Record 39 of 491

Title: Fanconi-Anemia-Associated Mutations Destabilize RAD51 Filaments and Impair Replication Fork Protection

Author(s): Zadorozhny, K (Zadorozhny, Karina); Sannino, V (Sannino, Vincenzo); Belan, O (Belan, Ondrej); Mlcouskova, J (Mlcouskova, Jarmila); Spirek, M (Spirek, Mario); Costanzo, V (Costanzo, Vincenzo); Krejci, L (Krejci, Lumir)

Source: CELL REPORTS **Volume:** 21 **Issue:** 2 **Pages:** 333-340 **DOI:** 10.1016/j.celrep.2017.09.062 **Published:** OCT 10 2017

Abstract: Fanconi anemia (FA) is a genetic disorder characterized by a defect in DNA interstrand crosslink (ICL) repair, chromosomal instability, and a predisposition to cancer. Recently, two RAD51 mutations were reported to cause an FA-like phenotype. Despite the tight association of FA/HR proteins with replication fork (RF) stabilization during normal replication, it remains unknown how FA-associated RAD51 mutations affect replication beyond ICL lesions. Here, we report that these mutations fail to protect nascent DNA from MRE11-mediated degradation during RF stalling in Xenopus laevis egg extracts. Reconstitution of DNA protection in vitro revealed that the defect arises directly due to altered RAD51 properties. Both mutations induce pronounced structural changes and RAD51 filament destabilization that is not rescued by prevention of ATP hydrolysis due to aberrant ATP binding. Our results further interconnect the FA pathway with DNA replication and provide mechanistic insight into the role of RAD51 in recombination-independent mechanisms of genome maintenance.

Accession Number: WOS:000412686100005

PubMed ID: 29020621

ISSN: 2211-1247

Record 40 of 491

Title: Fragmentation of Kr-N(+) clusters after electron impact ionization II. Long-time dynamics simulations of Kr-7(+) evolution and the role of initial electronic excitation

Author(s): Janecek, I (Janecek, Ivan); Stachon, M (Stachon, Martin); Gadea, FX (Gadea, Florent Xavier); Kalus, R (Kalus, Rene)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 37 **Pages:** 25423-25440 **DOI:** 10.1039/c7cp03940a **Published:** OCT 7 2017

Abstract: Long time simulations, up to 100 ns, have been performed for the fragmentation of Kr-7(+) clusters after electron impact ionization. They rely on DIM approaches and hybrid non-adiabatic dynamics combining mean field and decoherence driven either by Tully fewest switches (TFS) algorithm or through electronic amplitude (AMP) calculations. With both methods, for the first time, when the initial electronic excited state belongs to group II correlating to P-1/2 atomic ions, the fragmentation ratio in mainly monomer and dimer ions agrees very well with known experimental results. A complex non-adiabatic dynamics is found where initial neutral monomer evaporations due to gradual deexcitation over electronic states of group II are followed by a non-adiabatic transition across a wide energy gap of the spin-orbit origin to electronic states of group I. The resulting excess of kinetic energy causes the final fragmentation of charged intermediate fragments to stable ionic monomers or dimers. Characteristic times of these processes have been estimated. The kinetic energy distribution of the neutral and ionic monomers (the dominating final fragments) has been analyzed in detail. Interestingly they exhibit some signature of the initial excited electronic state which could allow for an experimental identification.

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PubMed ID: 28895597

ISSN: 1463-9076

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Record 41 of 491

Title: Adsorbate-driven cooling of carbene-based molecular junctions

Author(s): Foti, G (Foti, Giuseppe); Vazquez, H (Vazquez, Hector)

Source: BEILSTEIN JOURNAL OF NANOTECHNOLOGY **Volume:** 8 **Pages:** 2060-2068 **DOI:** 10.3762/bjnano.8.206 **Published:** OCT 2 2017

Abstract: We study the role of an NH2 adsorbate on the current-induced heating and cooling of a neighboring carbene-based molecular circuit. We use first-principles methods of inelastic tunneling transport based on density functional theory and non-equilibrium Green's functions to calculate the rates of emission and absorbtion of vibrations by tunneling electrons, the population of vibrational modes and the energy stored in them. We find that the charge rearrangement resulting from the adsorbate gates the carbene electronic structure and reduces the density of carbene states near the Fermi level as a function of bias. These effects result in the cooling of carbene modes at all voltages compared to the "clean" carbene-based junction. We also find that the direct influence of adsorbate states is significantly smaller and tends to heat adsorbate vibrations. Our results highlight the important role of molecular adsorbates not only on the electronic and elastic transport properties but also on the current-induced energy exchange and stability under bias of single-molecule circuits.

Accession Number: WOS:000412224500001

PubMed ID: 29090108

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922

ISSN: 2190-4286

Record 42 of 491

Title: Vapor Pressures and Thermophysical Properties of Dimethyl Carbonate, Diethyl Carbonate, and Dipropyl Carbonate

Author(s): Pokorny, V (Pokorny, Vaclav); Stejfa, V (Stejfa, Vojtech); Fulem, M (Fulem, Michal); Cervinka, C (Cervinka, Ctirad); Ruzicka, K (Ruzicka, Kvetoslav)

Source: JOURNAL OF CHEMICAL AND ENGINEERING DATA **Volume:** 62 **Issue:** 10 **Pages:** 3206-3215 **DOI:** 10.1021/acs.jced.7b00295 **Published:** OCT 2017

Abstract: In this work, a thermodynamic study of important industrial solvents, dimethyl carbonate (CAS RN: 616-38-6), diethyl carbonate (CAS RN: 105-58-8), and dipropyl carbonate (CAS RN: 623-96-1), is presented. The vapor pressure pressure measurements were performed using the static method in the temperature interval 238-308 K. Heat capacities of condensed phases were measured by Tian-Calvet calorimetry in the temperature interval 260-358 K. The phase behavior was investigated by DSC in the temperature interval 183-300 K. The thermodynamic properties in the ideal gaseous state were calculated using the methods of statistical thermodynamics based on calculated fundamental vibrational frequencies and molecular structure data. Calculated ideal-gas heat capacities and experimental data on vapor pressures, condensed phase heat capacities, and vaporization enthalpies were treated simultaneously to obtain a consistent thermodynamic description.

Accession Number: WOS:000413131800021

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ruzicka, Kvetoslav	B-1071-2008	0000-0001-9048-1036
Stejfa, Vojtech	G-9925-2018	0000-0002-2839-8546
Pokorny, Vaclav	O-7358-2017	0000-0003-4145-7982

ISSN: 0021-9568

Record 43 of 491

Title: Automatic Creation of Machine Learning Workflows with Strongly Typed Genetic Programming

Author(s): Kren, T (Kren, Tomas); Pilat, M (Pilat, Matin); Neruda, R (Neruda, Roman)

Source: INTERNATIONAL JOURNAL ON ARTIFICIAL INTELLIGENCE TOOLS **Volume:** 26 **Issue:** 5 **Special Issue:** SI **Article Number:** 1760020 **DOI:** 10.1142/S021821301760020X **Published:** OCT 2017

Abstract: Manual creation of machine learning ensembles is a hard and tedious task which requires an expert and a lot of time. In this work we describe a new version of the GP-ML algorithm which uses genetic programming to create machine learning workows (combinations of preprocessing, classification, and ensembles) automatically, using strongly typed genetic programming and asynchronous evolution. The current version improves the way in which the individuals in the genetic programming are created and allows for much larger workows. Additionally, we added new machine learning methods. The algorithm is compared to the grid search of the base methods and to its previous versions on a set of problems from the UCI machine learning repository.

Accession Number: WOS:000413237100006

Conference Title: 28th Annual IEEE International Conference on Tools with Artificial Intelligence (ICTAI)

Conference Date: NOV 06-08, 2016

Conference Location: San Jose, CA

Conference Sponsors: IEEE, Biol & Artificial Intelligence Fdn, IEEE Comp Soc

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Neruda, Roman	D-2442-2014	0000-0003-2364-5357

ISSN: 0218-2130

eISSN: 1793-6349

Record 44 of 491

Title: Genome mining reveals high incidence of putative lipopeptide biosynthesis NRPS/PKS clusters containing fatty acyl-AMP ligase genes inbiofilm-forming cyanobacteria

Author(s): Galica, T (Galica, Tomas); Hrouzek, P (Hrouzek, Pavel); Mares, J (Mares, Jan)

Source: JOURNAL OF PHYCOLOGY **Volume:** 53 **Issue:** 5 **Pages:** 985-998 **DOI:** 10.1111/jpy.12555 **Published:** OCT 2017

Abstract: Cyanobacterial lipopeptides have antimicrobial and antifungal bioactivities with potential for use in pharmaceutical research. However, due to their hemolytic activity and cytotoxic effects on human cells, they may pose a health issue if produced in substantial amounts in the environment. In bacteria, lipopeptides can be synthesized via several well-evidenced mechanisms. In one of them, fatty acyl-AMP ligase (FAAL) initiates biosynthesis by activation of a fatty acyl residue. We have performed a bioinformatic survey of the cyanobacterial genomic information available in the public databases for the presence of FAAL-containing non-ribosomal peptide synthetase/polyketide synthetase (NRPS/PKS) biosynthetic clusters, as a genetic basis for lipopeptide biosynthesis. We have identified 79 FAAL genes associated with various NRPS/PKS clusters in 16% of 376 cyanobacterial genomic assemblies available, suggesting that FAAL is frequently incorporated in NRPS/PKS biosynthetases. FAAL was present either as a stand-alone protein or fused either to NRPS or PKS. Such clusters were more frequent in derived phylogenetic lineages with larger genome sizes, which is consistent with the general pattern of NRPS/PKS pathways distribution. The putative lipopeptide clusters were more frequently found in genomes of cyanobacteria that live attached to surfaces and are capable of forming microbial biofilms. While lipopeptides are known in other bacterial groups to play a role in biofilm formation, motility, and colony expansion, their functions in cyanobacterial biofilms need to be tested experimentally. According to our data, benthic and terrestrial cyanobacteria should be the focus of a search for novel candidates for lipopeptide drug synthesis and the monitoring of toxic lipopeptide production.

Accession Number: WOS:000413167600007

PubMed ID: 28632895

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mares, Jan	B-2395-2009	0000-0002-5745-7023

ISSN: 0022-3646

eISSN: 1529-8817

Record 45 of 491

Title: Stability of housekeeping gene expression in Arabidopsis thaliana seedlings under differing macronutrient and hormonal conditions

Author(s): Soucek, P (Soucek, Premysl); Pavlu, J (Pavlu, Jaroslav); Medved'ova, Z (Medved'ova, Zuzana); Reinohl, V (Reinohl, Vilem); Brzobohaty, B (Brzobohaty, Bretislav)
Source: JOURNAL OF PLANT BIOCHEMISTRY AND BIOTECHNOLOGY **Volume:** 26 **Issue:** 4 **Pages:** 415-424 **DOI:** 10.1007/s13562-017-0403-0 **Published:** OCT 2017
Abstract: Recent progress in plant hormone and macronutrient research is largely associated with characterising the molecular mechanisms of their actions. Quantitative reverse transcription-PCR is a powerful technique that enables elucidation of regulatory relationships through quantifying transcript levels, but its reliability requires precise normalization. We compared eight Arabidopsis thaliana housekeeping genes for expression stability after treatment with cytokinins, auxins, ethylene and after macronutrient level manipulation. The expression stability of housekeeping genes in cytokinin series was studied in wide spectrum of plants treated with different adenine- and phenylurea-type cytokinins as well as in plants with controlled overexpression of agrobacterial isopentenyltransferase. NormFinder and geNorm software were used to predict a unique set of genes as best for particular hormone groups. Generally, 18S rRNA, GAPC, and ACT were confirmed as less stable; and UBQ10, UBC, and EF-1 alpha exhibited increased stability. Based on geNorm pairwise variation analysis, we confirmed accurate normalization required at least three reference genes.
Accession Number: WOS:000413808400005
ISSN: 0971-7811
eISSN: 0974-1275

Record 46 of 491

Title: Codiversification of gastrointestinal microbiota and phylogeny in passerines is not explained by ecological divergence
Author(s): Kropackova, L (Kropackova, Lucie); Tesicky, M (Tesicky, Martin); Albrecht, T (Albrecht, Tomas); Kubovciak, J (Kubovciak, Jan); Cizkova, D (Cizkova, Dagmar); Tomasek, O (Tomasek, Oldrich); Martin, JF (Martin, Jean-Francois); Bobek, L (Bobek, Lukas); Kralova, T (Kralova, Tereza); Prochazka, P (Prochazka, Petr); Kreisinger, J (Kreisinger, Jakub)
Source: MOLECULAR ECOLOGY **Volume:** 26 **Issue:** 19 **Pages:** 5292-5304 **DOI:** 10.1111/mec.14144 **Published:** OCT 2017
Abstract: Vertebrate gut microbiota (GM) is comprised of a taxonomically diverse consortium of symbiotic and commensal microorganisms that have a pronounced effect on host physiology, immune system function and health status. Despite much research on interactions between hosts and their GM, the factors affecting inter- and intraspecific GM variation in wild populations are still poorly known. We analysed data on faecal microbiota composition in 51 passerine species (319 individuals) using Illumina MiSeq sequencing of bacterial 16S rRNA (V3-V4 variable region). Despite pronounced interindividual variation, GM composition exhibited significant differences at the interspecific level, accounting for approximately 20%-30% of total GM variation. We also observed a significant correlation between GM composition divergence and host's phylogenetic divergence, with strength of correlation higher than that of GM vs. ecological or life history traits and geographic variation. The effect of host's phylogeny on GM composition was significant, even after statistical control for these confounding factors. Hence, our data do not support codiversification of GM and passerine phylogeny solely as a by-product of their ecological divergence. Furthermore, our findings do not support that GM vs. host's phylogeny codiversification is driven primarily through trans-generational GM transfer as the GM vs. phylogeny correlation does not increase with higher sequence similarity used when delimiting operational taxonomic units. Instead, we hypothesize that the GM vs. phylogeny correlation may arise as a consequence of interspecific divergence of genes that directly or indirectly modulate composition of GM.
Accession Number: WOS:000413375500031
PubMed ID: 28401612
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Albrecht, Tomas	A-1130-2011	
Tomasek, Oldrich	A-6725-2012	0000-0002-2657-5916
Prochazka, Petr	A-9727-2008	0000-0001-9385-4547
Kreisinger, Jakub	H-4020-2011	
Tesicky, Martin	L-3370-2017	0000-0001-8097-5331
Kropackova, Lucie		0000-0003-2180-5281
Albrecht, Tomas		0000-0002-9213-0034

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Record 47 of 491

Title: Quantitative Determination of Ala-Ala Conformer Ratios in Solution by Decomposition of Raman Optical Activity Spectra
Author(s): Jungwirth, J (Jungwirth, Jakub); Sebestik, J (Sebestik, Jaroslav); Safarik, M (Safarik, Martin); Kapitan, J (Kapitan, Josef); Bour, P (Bour, Petr)
Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 121 **Issue:** 38 **Pages:** 8956-8964 **DOI:** 10.1021/acs.jpcb.7b07154 **Published:** SEP 28 2017
Abstract: Raman optical activity (ROA) spectroscopy combined with quantum-chemical simulations is a sensitive method to determine the absolute configuration and conformation of chiral molecules in solutions. However, the precision of this approach varies for different systems. In the present study, the reliability and numerical stability of decomposing experimental spectra into calculated subspectra is tested on the Ala-Ala dipeptide. Molecular dynamics (MD) snapshots of Ala-Ala/water clusters are averaged to account for solvent effects and molecular flexibility. Multiple experiments with protonated, zwitterionic, and deprotonated dipeptide forms and natural and d(2)- and d(8)-isotopically labeled dipeptides are used to verify the results and estimate the overall accuracy. Although the precision is still limited by experimental noise and computational error, a very close match between the observed and theoretical spectral shapes has been achieved. This enabled quantitative determination of conformer populations with a typical dispersion of 10%. The spectroscopy also demonstrated how the conformation depends on pH. The ROA results were more consistent than the Raman ones. Typically, the ROA analysis was more resistant to artifacts in the experiment, such as incomplete baseline subtraction. Conformer ratios predicted by MD agree fairly but not fully with the experimental ones. This indicates minor deficiencies in the Amber force field, particularly for the protonated dipeptide. Overall, the combination of ROA experiment and computational chemistry appears to be a robust tool providing deep insight into molecular structure.
Accession Number: WOS:000412150700009
PubMed ID: 28853886
ISSN: 1520-6106

Record 48 of 491

Title: Physical properties of the tetragonal CuMnAs: A first-principles study
Author(s): Maca, F (Maca, F.); Kudrnovsky, J (Kudrnovsky, J.); Drchal, V (Drchal, V.); Carva, K (Carva, K.); Balaz, P (Balaz, P.); Turek, I (Turek, I.)
Source: PHYSICAL REVIEW B **Volume:** 96 **Issue:** 9 **Article Number:** 094406 **DOI:** 10.1103/PhysRevB.96.094406 **Published:** SEP 6 2017
Abstract: Electronic, magnetic, and transport properties of the antiferromagnetic (AFM) CuMnAs alloy with tetragonal structure, promising for the AFM spintronics, are studied from first principles using the Vienna ab initio simulation package. We investigate the site occupation of sublattices and the lattice parameters of three competing phases. We analyze the factors that determine which of the three conceivable structures will prevail. We then estimate formation energies of possible defects for the experimentally prepared lattice structure. Mn-Cu and Cu-Mn antisites as well as Mn <-> Cu swaps and vacancies on Mn or Cu sublattices were identified as possible candidates for defects in CuMnAs. We find that the interactions of the growing thin film with the substrate and with vacuum as well as the electron correlations are important for the phase stability while the effect of defects is weak. In the next step, using the tight-binding linear muffin-tin orbital method for the experimental structure, we estimate transport properties for systems containing defects with low formation energies. Finally, we determine the exchange interactions and estimate the Neel temperature of the AFM-CuMnAs alloy using the Monte Carlo approach. A good agreement of the calculated resistivity and Neel temperature with experimental data makes it possible to draw conclusions concerning the competing phases.
Accession Number: WOS:000409428500004
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Balaz, Pavel	M-9510-2015	0000-0003-0016-9271
Carva, Karel	A-3703-2008	0000-0002-2275-1986

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Record 49 of 491

Title: Transcriptome of barley under three different heavy metal stress reaction
Author(s): Kintlova, M (Kintlova, Martina); Blavet, N (Blavet, Nicolas); Cegan, R (Cegan, Radim); Hobza, R (Hobza, Roman)
Source: GENOMICS DATA **Volume:** 13 **Pages:** 15-17 **DOI:** 10.1016/j.gdata.2017.05.016 **Published:** SEP 2017

Abstract: In the present study, we used Illumina sequencing technology (HiSeq 2000) to sequence the transcriptome of barley (Hordeum vulgare L., cv. Morex) under three different heavy metal stress conditions: copper, zinc and cadmium. For each of those metals, the concentration causing a 50% inhibitory effect for root growth (EC50) was determined. We sequenced the total RNA of both roots and shoots from barley with and without heavy metal treatments in three replicates. Raw reads of the transcriptome project have been deposited in NCBI's BioProject accession number PRJNA382490. The obtained transcriptomic data will be useful for further studies focusing on heavy metal tolerance and comparative transcriptome analysis in barley.

Accession Number: WOS:000415937000006

PubMed ID: 28626638

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cegan, Radim	H-1892-2014	0000-0002-6789-6564
Blavet, Nicolas		0000-0003-2199-9119

ISSN: 2213-5960

Record 50 of 491

Title: Exploring the stability and reactivity of Ni2P and Mo2C catalysts using ab initio atomistic thermodynamics and conceptual DFT approaches

Author(s): Morales-Garcia, A (Morales-Garcia, Angel); He, JJ (He, Junjie); Lyu, P (Lyu, Pengbo); Nachtigall, P (Nachtigall, Petr)

Source: BIOMASS CONVERSION AND BIOREFINERY **Volume:** 7 **Issue:** 3 **Pages:** 377-383 **DOI:** 10.1007/s13399-017-0278-2 **Published:** SEP 2017

Abstract: The stability and reactivity of Mo2C and Ni2P surfaces with different terminations are systematically investigated by means of ab initio atomistic thermodynamics and conceptual DFT approaches as a function of the chemical potential (mu). Five surfaces labeled as (001)-Mo-1, (110)-Mo/C, (001)-Ni3P2, (001)-Ni3P2-P, and (001)-Ni3P1 emerge as the most stable ones for Mo2C and Ni2P catalysts depending on mu (C) and mu (P), respectively. The Fukui function, a reactivity descriptor, reveals that the metal atoms interact preferentially with nucleophilic adsorbates such as H2S. Here, our study predicts that a high concentration of C and P atoms on the surface reduces the catalytic activity where nucleophilic species are involved. The qualitative agreement between the nucleophilic Fukui function (f (+)) and the adsorption energies indicates that the Ni2P catalyst is, in general, more reactive than Mo2C catalyst. This study may help to improve and optimize the catalytic processes, such as the hydrogenations HDO and HDS, where Mo2C and Ni2P catalysts are involved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Nachtigall, Petr	A-6220-2013	0000-0002-1628-7275

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Page 2 (Records 51 -- 100)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 51 of 491

Title: Dissipative particle dynamics simulations of polyelectrolyte self-assemblies. Methods with explicit electrostatics

Author(s): Lisal, M (Lisal, Martin); Sindelka, K (Sindelka, Karel); Sucha, L (Sucha, Lucie); Limpouchova, Z (Limpouchova, Zuzana); Prochazka, K (Prochazka, Karel)

Source: POLYMER SCIENCE SERIES C **Volume:** 59 **Issue:** 1 **Pages:** 77-101 **DOI:** 10.1134/S1811238217010052 **Published:** SEP 2017

Abstract: This feature article is addressed to a broad community of polymer scientists, both theoreticians and experimentalists. We present several examples of our dissipative particle dynamics (DPD) simulations of selfand co-assembling polyelectrolyte systems to illustrate the power of DPD. In the first part, we briefly outline basic principles of DPD. Special emphasis is placed on the incorporation of explicit electrostatic forces into DPD, on their calibration with respect to the soft repulsion forces and on the use of DPD for studying the self-assembly of electrically charged polymer systems. At present, the method with explicit electrostatics is being used in a number of studies of the behavior of single polyelectrolyte chains, their interaction with other components of the system, etc. However, in DPD studies of self-assembly, which require high numbers of chains, only a few research groups use explicit electrostatics. Most studies of polyelectrolyte self-assembly are based on the "implicit solvent ionic strength" approach, which completely ignores the long-range character of electrostatic interactions, because their evaluation complicates and considerably slows down the DPD simulation runs. We aim at the analysis of the impact of explicit electrostatics on simulation results.

Accession Number: WOS:000408116600009

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Limpouchova, Zuzana	C-7791-2013	0000-0002-2290-1358
Lisal, Martin	A-8176-2011	0000-0001-8005-7143
Sindelka, Karel		0000-0003-3925-924X

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Record 52 of 491

Title: Enzyme Tunnels and Gates As Relevant Targets in Drug Design

Author(s): Marques, SM (Marques, Sergio M.); Daniel, L (Daniel, Lukas); Buryska, T (Buryska, Tomas); Prokop, Z (Prokop, Zbynek); Brezovsky, J (Brezovsky, Jan); Damborsky, J (Damborsky, Jiri)

Source: MEDICINAL RESEARCH REVIEWS **Volume:** 37 **Issue:** 5 **Pages:** 1095-1139 **DOI:** 10.1002/med.21430 **Published:** SEP 2017

Abstract: Many enzymes contain tunnels and gates that are essential to their function. Gates reversibly switch between open and closed conformations and thereby control the traffic of small molecules-substrates, products, ions, and solvent molecules-into and out of the enzyme's structure via molecular tunnels. Many transient tunnels and gates undoubtedly remain to be identified, and their functional roles and utility as potential drug targets have received comparatively little attention. Here, we describe a set of general concepts relating to the structural properties, function, and classification of these interesting structural features. In addition, we highlight the potential of enzyme tunnels and gates as targets for the binding of small molecules. The different types of binding that are possible and the potential pharmacological benefits of such targeting are discussed. Twelve examples of ligands bound to the tunnels and/or gates of clinically relevant enzymes are used to illustrate the different binding modes and to explain some new strategies for drug design. Such strategies could potentially help to overcome some of the problems facing medicinal chemists and lead to the discovery of more effective drugs. (C) 2016 Wiley Periodicals, Inc. Med. Res. Rev., 37, No. 5, 1095-1139, 2017

Accession Number: WOS:000406877600003

PubMed ID: 27957758

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Brezovsky, Jan	C-8290-2012	0000-0001-9677-5078
Marques, Sergio	H-8685-2012	0000-0002-6281-7505
Daniel, Lukas		0000-0003-2502-9224
Prokop, Zbynek		0000-0001-9358-4081

ISSN: 0198-6325

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Record 53 of 491

Title: Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality

Author(s): Timr, S (Timr, Stepan); Pleskot, R (Pleskot, Roman); Kadlec, J (Kadlec, Jan); Kohagen, M (Kohagen, Miriam); Magarkar, A (Magarkar, Aniket); Jungwirth, P (Jungwirth, Pavel)

Source: ACS CENTRAL SCIENCE **Volume:** 3 **Issue:** 8 **Pages:** 868-874 **DOI:** 10.1021/acscentsci.7b00210 **Published:** AUG 23 2017

Abstract: Recoverin is a neuronal calcium sensor involved in vision adaptation that reversibly associates with cellular membranes via its calcium-activated myristoyl switch. While experimental evidence shows that the myristoyl group significantly enhances membrane affinity of this protein, molecular details of the binding process are still under debate. Here, we present results of extensive molecular dynamics simulations of recoverin in the proximity of a phospholipid bilayer. We capture multiple events of spontaneous membrane insertion of the myristoyl moiety and confirm its critical role in the membrane binding. Moreover, we observe that the binding strongly depends on the conformation of the N-terminal domain. We propose that a suitable conformation of the N-terminal domain can be stabilized by the disordered C-terminal segment or by binding of the target enzyme, i.e., rhodopsin kinase. Finally, we find that the presence of negatively charged lipids in the bilayer stabilizes a physiologically functional orientation of the membrane-bound recoverin.

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PubMed ID: 28852701

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Pleskot, Roman	F-7774-2014	0000-0003-0436-9748
Timr, Stepan		0000-0002-5824-4476
Kadlec, Jan		0000-0003-2477-3633

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Record 54 of 491

Title: Hyaluronan random coils in electrolyte solutions-a molecular dynamics study

Author(s): Ingr, M (Ingr, Marek); Kutalkova, E (Kutalkova, Eva); Hrncirik, J (Hrncirik, Josef)

Source: CARBOHYDRATE POLYMERS **Volume:** 170 **Pages:** 289-295 **DOI:** 10.1016/j.carbpol.2017.04.054 **Published:** AUG 15 2017

Abstract: A computational method of modeling random coils of hyaluronan was developed based on the molecular dynamics simulations. An oligosaccharide of 48 monosaccharide units was equilibrated within a 70-100 ns simulation and randomly chosen pieces of this molecule from different simulation frames were combined to constitute a long polysaccharide chain, both for hyaluronan and its non-ionic analog containing glucose instead of glucuronic acid. The dihedral angles of the glycoside connections of the pieces obeyed the statistics, deduced from the simulation. The simulations were performed at various concentrations of NaCl and MgCl2. The calculated radii of gyration show a striking agreement with experimental data from the literature and indicate a key importance of the polymer-ion interactions for the random-coil conformation, but a low influence of the excluded volume of the chain and the carboxylate-groups repulsion. The method has thus the potential to become a versatile tool of modeling macromolecules of various semirigid polymers. (C) 2017 Elsevier Ltd. All rights reserved.

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PubMed ID: 28521999

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ingr, Marek	E-2478-2015	0000-0001-6741-9955
Kutalkova, Eva		0000-0003-3538-4019

ISSN: 0144-8617
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Record 55 of 491

Title: Development of 2-Methoxyhuprine as Novel Lead for Alzheimer's Disease Therapy

Author(s): Mezeiova, E (Mezeiova, Eva); Korabecny, J (Korabecny, Jan); Sepsova, V (Sepsova, Vendula); Hrabinova, M (Hrabinova, Martina); Jost, P (Jost, Petr); Muckova, L (Muckova, Lubica); Kucera, T (Kucera, Tomas); Dolezal, R (Dolezal, Rafael); Misik, J (Misik, Jan); Spilovska, K (Spilovska, Katarina); Pham, NL (Ngoc Lam Pham); Pokrievkova, L (Pokrievkova, Lucia); Roh, J (Roh, Jaroslav); Jun, D (Jun, Daniel); Soukup, O (Soukup, Ondrej); Kaping, D (Kaping, Daniel); Kuca, K (Kuca, Kamil)

Source: MOLECULES **Volume:** 22 **Issue:** 8 **Article Number:** 1265 **DOI:** 10.3390/molecules22081265 **Published:** AUG 2017

Abstract: Tacrine (THA), the first clinically effective acetylcholinesterase (AChE) inhibitor and the first approved drug for the treatment of Alzheimer's disease (AD), was withdrawn from the market due to its side effects, particularly its hepatotoxicity. Nowadays, THA serves as a valuable scaffold for the design of novel agents potentially applicable for AD treatment. One such compound, namely 7-methoxytacrine (7-MEOTA), exhibits an intriguing profile, having suppressed hepatotoxicity and concomitantly retaining AChE inhibition properties. Another interesting class of AChE inhibitors represents Huprines, designed by merging two fragments of the known AChE inhibitors-THA and (-)-huperzine A. Several members of this compound family are more potent human AChE inhibitors than the parent compounds. The most promising are so-called huprines X and Y. Here, we report the design, synthesis, biological evaluation, and in silico studies of 2-methoxyhuprine that amalgamates structural features of 7-MEOTA and huprine Y in one molecule.

Accession Number: WOS:000408602900030

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Jun, Daniel	S-8647-2017	0000-0002-0882-6304
Roh, Jaroslav	S-7863-2017	0000-0003-4698-8379
Kuca, Kamil		0000-0001-9664-1109
Sepsova, Vendula		0000-0002-6445-2669
Korabecny, Jan		0000-0001-6977-7596
Hrabinova, Martina		0000-0002-9428-4109

ISSN: 1420-3049

Record 56 of 491

Title: Structure and Dynamics of Alginate Gels Cross-Linked by Polyvalent Ions Probed via Solid State NMR Spectroscopy

Author(s): Brus, J (Brus, Jiri); Urbanova, M (Urbanova, Martina); Czernek, J (Czernek, Jiri); Pavelkova, M (Pavelkova, Miroslava); Kubova, K (Kubova, Katerina); Vyslouzil, J (Vyslouzil, Jakub); Abbrent, S (Abbrent, Sabina); Konefal, R (Konefal, Rafal); Horsky, J (Horsky, Jiri); Vetchy, D (Vetchy, David); Vyslouzil, J (Vyslouzil, Jan); Kulich, P (Kulich, Pavel)

Source: BIOMACROMOLECULES **Volume:** 18 **Issue:** 8 **Pages:** 2478-2488 **DOI:** 10.1021/acs.biomac.7b00627 **Published:** AUG 2017

Abstract: Alginate gels are an outstanding biomaterial widely applicable in tissue engineering, medicine, and pharmacy agent delivery, respectively. This contribution provides new and comrehensive into the atomic-resolution structure for cell transplantation, wound healing and efficient bioactive agent delivery, respectively. This contribution provides new and comrehensive insight into the atomic-resolution structure and dynamics of polyvalent ion-cross-linked alginate gels in microbead formulations. By applying various advanced solid-state NMR (ssNMR) spectroscopy techniques, we verified the homogeneous distribution of the cross-linking ions in the alginate gels and the high degree of ion exchange. We also established that the two-component character of the alginate gels arises from the concentration fluctuations of residual water molecules that are preferentially localized along polymer chains containing abundant mannuronic acid (M) residues. These hydrated M-rich blocks tend to self-aggregate into subnanometer domains. The resulting coexistence of two types of alginate chains differing in segmental dynamics was revealed by H-1-C-13 dipolar profile analysis, which indicated that the average fluctuation angles of the stiff and mobile alginate segments were about 5-9 degrees or 30 degrees, respectively. Next, the C-13 CP/MAS NMR spectra indicated that the alginate polymer microstructure was strongly dependent on the type of cross-linking ion. The polymer chain regularity was determined to systematically decrease as the cross linking ion radius decreased. Consistent with the H-1-H-1 correlation spectra, regular structures were found for the gels cross linked by relatively large alkaline earth cations (Ba2+, Sr2+, or Ca2+), whereas the alginate chains cross-linked by bivalent transition metal ions (Zn") and trivalent metal cations (Al3+) exhibited significant irregularities. Notably, however, the observed disordering of the alginate chains was exclusively attributed to the M residues, whereas the structurally well-defined gels all contained guluronic acid (G) residues. Therefore, a key role of the units in M-rich blocks as mediators promoting the self assembly of alginate chains was experimentally confirmed. Finally, combining 2D Al-27 3Q/MAS NMR spectroscopy with density functional theory (DFT) calculations provided previously unreported insight into the structure of the Al3+ cross-linking centers. Notably, even with a low residual amount of water, these cross-linking units adopt exclusively 6-fold octahedral coordination and exhibit significant motion, which considerably reduces quadrupolar coupling constants. Thus, the experimental strategy presented in this study provides a new perspective on cross-linked alginate structure and dynamics for which high-quality diffraction data at the atomic resolution level are inherently unavailable.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Czernek, Jiri	H-6708-2014	
Urbanova, Martina	G-9793-2014	0000-0003-1316-6395
Konefal, Rafal	G-5886-2014	0000-0003-4568-4891
Abbrent, Sabina	M-9812-2014	
Horsky, Jiri	G-3442-2014	
Brus, Jiri	G-3459-2014	
Kubova, Katerina		0000-0002-4970-2084

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Record 57 of 491

Title: Noncovalent Interactions by Fixed-Node Diffusion Monte Carlo: Convergence of Nodes and Energy Differences vs Gaussian Basis-Set Size

Author(s): Dubecky, M (Dubecky, Matus)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 13 **Issue:** 8 **Pages:** 3626-3635 **DOI:** 10.1021/acs.jctc.7b00537 **Published:** AUG 2017

Abstract: Convergence of fixed-node (FN) shape and FN diffusion Monte Carlo (FNDMC) interaction energies is studied vs the Gaussian basis set saturation level in HF and CH4 dimers and one-determinant Slater-Jastrow trial wave functions (Psi(T)). The tested 25 distinct basis sets obtained by stepwise trimming of aug-VDZ and aug-VTZ bases suggest minimum basis set requirements to achieve reasonable results. A single selected trimmed basis set, about 2 times smaller in size than aug-VTZ, is extensively tested on a set of 12 noncovalent complexes including formic acid dimer, benzene-methane, or coronene-H2. The results indicate that equivalent noncovalent FNDMC energy differences are available at costs lower than assumed before. Additional insights from electron density differences and comparison of dimer vs monomer Psi(T) nodes explain this observation.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dubecky, Matus	P-1720-2016	

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Record 58 of 491

Title: Long terminal repeats power evolution of genes and gene expression programs in mammalian oocytes and zygotes

Author(s): Franke, V (Franke, Vedran); Ganesh, S (Ganesh, Sravya); Karlic, R (Karlic, Rosa); Malik, R (Malik, Radek); Pasulka, J (Pasulka, Josef); Horvat, F (Horvat, Filip); Kuzman, M (Kuzman, Maja); Fulka, H (Fulka, Helena); Cernohorska, M (Cernohorska, Marketa); Urbanova, J (Urbanova, Jana); Svobodova, E (Svobodova, Eliska); Ma, J (Ma, Jun); Suzuki, Y (Suzuki, Yutaka); Aoki, F (Aoki, Fugaku); Schultz, RM (Schultz, Richard M.); Vlahovicek, K (Vlahovicek, Kristian); Svoboda, P (Svoboda, Petr)

Source: GENOME RESEARCH **Volume:** 27 **Issue:** 8 **Pages:** 1384-1394 **DOI:** 10.1101/gr.216150.116 **Published:** AUG 2017

Abstract: Retrotransposons are "copy-and-paste" insertional mutagens that substantially contribute to mammalian genome content. Retrotransposons often carry long terminal repeats (LTRs) for retrovirus-like reverse transcription and integration into the genome. We report an extraordinary impact of a group of LTRs from the mammalian endogenous retrovirus-related ERVL retrotransposon class on gene expression in the germline and beyond. In mouse, we identified more than 800 LTRs from ORR1, MT, MT2, and MLT families, which resemble mobile gene-remodeling platforms that supply promoters and first exons. The LTR-mediated gene remodeling also extends to hamster, human, and bovine oocytes. The LTRs function in a stage specific manner during the oocyte-to-embryo transition by activating transcription, altering protein-coding sequences, producing noncoding RNAs, and even supporting evolution of new protein-coding genes. These functions result, for example, in recycling processed pseudogenes into mRNAs or lncRNAs with regulatory roles. The functional potential of the studied LTRs is even higher, because we show that dormant LTR promoter activity can rescue loss of an essential upstream promoter. We also report a novel protein-coding gene evolution-D6Ertd527e-in which an MT LTR provided a promoter and the 5' exon with a functional start codon while the bulk of the protein-coding sequence evolved through a CAG repeat expansion. Altogether, ERVL LTRs provide molecular mechanisms for stochastically scanning, rewiring, and recycling genetic information on an extraordinary scale. ERVL LTRs thus offer means for a comprehensive survey of the genome's expression potential, tightly intertwining with gene expression and evolution in the germline.

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PubMed ID: 28522611

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vlahovicek, Kristian	D-9661-2011	0000-0002-5705-2464
Svoboda, Petr	G-3890-2012	0000-0002-4370-3705
Horvat, Filip	S-1904-2017	0000-0002-1896-7645
Cernohorska, Marketa		0000-0001-9053-8928
Franke, Vedran		0000-0003-3606-6792

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Record 59 of 491

Title: A meta-heuristic based goal-selection strategy for mobile robot search in an unknown environment

Author(s): Kulich, M (Kulich, Miroslav); Miranda-Bront, JJ (Jose Miranda-Bront, Juan); Preucil, L (Preucil, Libor)

Source: COMPUTERS & OPERATIONS RESEARCH **Volume:** 84 **Pages:** 178-187 **DOI:** 10.1016/j.cor.2016.04.029 **Published:** AUG 2017

Abstract: The single-robot search problem in an unknown environment is defined as the problem of finding a stationary object in the environment whose map is not known a priori. Compared to exploration, the only difference lies in goal selection as the objectives of search and exploration are dissimilar, i.e. a trajectory that is optimal in exploration does not necessarily minimize the expected value of the time to find an object along it. For this reason, in this paper we extend the preliminary ideas presented in Kulich et al. [1] to a general framework that accounts for the particular characteristics of the search problem. Within this framework, an important decision involved in the determination of the trajectory can be formulated as an instance of the Graph Search Problem (GSP), a generalization of the well-known Traveling Deliveryman Problem (TDP) which has not received much attention in the literature. We developed a tailored Greedy Randomized Adaptive Search Procedure (GRASP) meta-heuristic for the GSP, which generates good quality solutions in very short computing times and is incorporated in the overall framework. The proposed approach produces very good results in a simulation environment, showing that it is feasible from a computational standpoint and the proposed strategy outperforms the standard approaches. (C) 2016 Elsevier Ltd. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kulich, Miroslav	L-3465-2013	0000-0002-0997-5889
Miranda Bront, Juan Jose		0000-0001-9125-7028

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Record 60 of 491

Title: Magnetic properties of the CrMnFeCoNi high-entropy alloy

Author(s): Schneeweiss, O (Schneeweiss, Oldrich); Friak, M (Friak, Martin); Dudova, M (Dudova, Marie); Holec, D (Holec, David); Sob, M (Sob, Mojmir); Kriegner, D (Kriegner, Dominik); Holy, V (Holy, Vaclav); Beran, P (Beran, Premysl); George, EP (George, Easo P.); Neugebauer, J (Neugebauer, Joerg); Dlouhy, A (Dlouhy, Antonin)

Source: PHYSICAL REVIEW B **Volume:** 96 **Issue:** 1 **Article Number:** 014437 **DOI:** 10.1103/PhysRevB.96.014437 **Published:** JUL 28 2017

Abstract: We present experimental data showing that the equiatomic CrMnFeCoNi high-entropy alloy undergoes two magnetic transformations at temperatures below 100 K while maintaining its fcc structure down to 3 K. The first transition, paramagnetic to spin glass, was detected at 93 K and the second transition of the ferromagnetic type occurred at 38 K. Field-assisted cooling below 38 K resulted in a systematic vertical shift of the hysteresis curves. Strength and direction of the associated magnetization bias was proportional to the strength and direction of the cooling field and shows a linear dependence with a slope of 0.006 +/- 0.001 emu/T. The local magnetic moments of individual atoms in the CrMnFeCoNi quinary fcc random solid solution were investigated by ab initio (electronic density functional theory) calculations. Results of the numerical analysis suggest that, irrespective of the initial configuration of local magnetic moments, the magnetic moments associated with Cr atoms align antiferromagnetically with respect to a cumulative magnetic moment of their first coordination shell. The ab initio calculations further showed that the magnetic moments of Fe and Mn atoms remain strong (between 1.5 and 2 mu(B)), while the local moments of Ni atoms effectively vanish. These results indicate that interactions of Mn- and/or Fe-located moments with the surrounding magnetic structure account for the observed macroscopic magnetization bias.

Accession Number: WOS:000411905400003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Holy, Vaclav	E-1508-2017	0000-0002-0370-6928
Beran, Premysl	F-8855-2012	0000-0002-1217-3131
Kriegner, Dominik	C-6225-2013	0000-0001-6961-6581

ISSN: 2469-9950

eISSN: 2469-9969

Record 61 of 491

Title: Assembling of bis(tpy)fluorenes with Zn2+ and Fe2+ ions into metallo-supramolecular polymers with highly efficient white-light emission

Author(s): Hrma, M (Hrma, Martin); Sichova, K (Sichova, Kristyna); Svoboda, J (Svoboda, Jan); Vohlidal, J (Vohlidal, Jiri)

Source: POLYMER **Volume:** 122 **Pages:** 22-33 **DOI:** 10.1016/j.polymer.2017.06.037 **Published:** JUL 28 2017

Abstract: Three fully pi-conjugated bisterpyridines with fluorene unit in the central block were synthetized using the Suzuki-Miyaura coupling and transformed to corresponding conjugated metallo-supramolecular polymers (MSPs) with Zn2+ or Fe2+ ions. Assembling course of MSPs was investigated by absorption and emission spectroscopy, size-exclusion chromatography and viscometric measurements. Two systems with Zn2+ ions showed white emission with high quantum yields of fluorescence. The constitutional dynamics of Zn-polymers is fast while that of Fe-polymers is as slow that it allows effective separation of the polymer in SEC columns. Electronic spectra and SEC measurements proved that excess of Fe2+ ions results in their end-capping by these ions and shortening of the polymer chains. The phenomenon of shortening of the polymer chains by surplus of metal ions was additionally confirmed by viscometry measurements for both ion-couplers, which provides us new awareness about the length of MSPs with Zn2+ ions. (C) 2017 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000406822200003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sichova, Kristyna	P-4123-2017	0000-0002-9882-9057
Svoboda, Jan	E-4750-2014	0000-0002-4989-4274
Vohlidal, Jiri		0000-0002-9412-2548

ISSN: 0032-3861
eISSN: 1873-2291

Record 62 of 491

Title: Effect of Nitrogen Doping on Glass Transition and Electrical Conductivity of [EMIM][PF6] Ionic Liquid Encapsulated in a Zigzag Carbon Nanotube

Author(s): Taherkhani, F (Taherkhani, Farid); Minofar, B (Minofar, Babak)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 121 **Issue:** 29 **Pages:** 15493-15508 **DOI:** 10.1021/acs.jpcc.7b00911 **Published:** JUL 27 2017

Abstract: Molecular level understanding of the properties of ionic liquids inside nanopores is needed in order to use ionic liquids for many applications such as electrolytes for energy storage in electric double-layer capacitors and dye-sensitized solar cells for conversion of solar energy. In this study, classical molecular dynamics (MD) simulations have been performed to investigate the radial distribution, glass transition, ionic transfer number, and electrical conductivity of the ionic liquid 1-ethyl-3-methylimidazolium hexafluorophosphate [EMIM][PF6] ionic liquid encapsulated in carbon nanotube (CNT). The effect of nitrogen as a doping element in CNT on these properties of [EMIM][PF6] was also investigated by MD simulation, and the configurational entropy of [EMIM][PF6] encapsulated in CNT was calculated in absence and presence of nitrogen: as a doping element. The configurational entropy of [EMIM][PF6] encapsulated in CNT is nonmonotonic versus temperature in both the presence absence of nitrogen doping. The glass transition of [EMIM][PF6] encapsulated in CNT is shifted to high temperature with doped nitrogen. The Green-Kubo formalism was used to calculate the ionic transfer number of [EMIM][PF6] encapsulated in CNT. Ionic transfer numbers show a maximum peak for cation transfer and a minimum peak for anion transfer with temperature. Electrical conductivity of [EMIM][PF6] encapsulated in CNT decreases with increasing temperature in, the presence of doped nitrogen and increases in absence of nitrogen. The cationic conductivity also increases with temperature in the presence vs absence of nitrogen doping. The MD findings for electrical conductivity and glass transition with temperature are in good agreement with available experimental data. The MD data shed new light on the effect of nitrogen doping on the mechanism of ion transfer. In the presence of nitrogen, ion transfer uses a hydrogen bonding mechanism, and in its absence, ion transfer uses a diffusion mechanism in which the cation has a significant effect on ion transfer and electrical conductivity.

Accession Number: WOS:000406726200002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Taherkhani, Farid		0000-0003-2433-4964

ISSN: 1932-7447

Record 63 of 491

Title: Transport properties of iron at Earth's core conditions: The effect of spin disorder

Author(s): Drchal, V (Drchal, V.); Kudrnovsky, J (Kudrnovsky, J.); Wagenknecht, D (Wagenknecht, D.); Turek, I (Turek, I.); Khmelevskyi, S (Khmelevskyi, S.)

Source: PHYSICAL REVIEW B **Volume:** 96 **Issue:** 2 **Article Number:** 024432 **DOI:** 10.1103/PhysRevB.96.024432 **Published:** JUL 21 2017

Abstract: The electronic and thermal transport properties of the Earth's core are crucial for many geophysical models such as the geodynamo model of the Earth's magnetic field and of its reversals. Here we show, by considering bcc iron and an iron-rich iron-silicon alloy as a representative of the Earth's core composition and applying first-principles modeling, that the spin disorder at the Earth's core conditions not considered previously provides an essential contribution, of order 20 mu Omega cm, to the electrical resistivity. This value is comparable in magnitude with the electron-phonon and with the recently estimated electron-electron scattering contributions. The origin of the spin-disorder resistivity (SDR) consists of the existence of fluctuating local moments that are stabilized at high temperatures by the magnetic entropy even at pressures at which the ground state of iron is nonmagnetic. We find that electron-phonon and SDR contributions are not additive at high temperatures. We thus observe a large violation of the Matthiessen rule, not common in conventional metallic alloys at ambient conditions.

Accession Number: WOS:000406034800006

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Wagenknecht, David	P-4165-2017	0000-0003-1927-9702
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Khmelevskyi, Sergii	T-1192-2017	0000-0001-5630-7835

ISSN: 2469-9950
eISSN: 2469-9969

Record 64 of 491

Title: Highly-conducting molecular circuits based on antiaromaticity

Author(s): Fujii, S (Fujii, Shintaro); Marques-Gonzalez, S (Marques-Gonzalez, Santiago); Shin, JY (Shin, Ji-Young); Shinokubo, H (Shinokubo, Hiroshi); Masuda, T (Masuda, Takuya); Nishino, T (Nishino, Tomoaki); Arasu, NP (Arasu, Narendra P.); Vazquez, H (Vazquez, Hector); Kiguchi, M (Kiguchi, Manabu)

Source: NATURE COMMUNICATIONS **Volume:** 8 **Article Number:** 15984 **DOI:** 10.1038/ncomms15984 **Published:** JUL 19 2017

Abstract: Aromaticity is a fundamental concept in chemistry. It is described by Huckel's rule that states that a cyclic planar pi-system is aromatic when it shares 4n+2 pi-electrons and antiaromatic when it possesses 4n pi-electrons. Antiaromatic compounds are predicted to exhibit remarkable charge transport properties and high redox activities. However, it has so far only been possible to measure compounds with reduced aromaticity but not antiaromatic species due to their energetic instability. Here, we address these issues by investigating the single-molecule charge transport properties of a genuinely antiaromatic compound, showing that antiaromaticity results in an order of magnitude increase in conductance compared with the aromatic counterpart. Single-molecule current-voltage measurements and ab initio transport calculations reveal that this results from a reduced energy gap and a frontier molecular resonance closer to the Fermi level in the antiaromatic species. The conductance of the antiaromatic complex is further modulated electrochemically, demonstrating its potential as a high-conductance transistor.

Accession Number: WOS:000405816100001

PubMed ID: 28722006

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kiguchi, Manabu	F-2856-2013	
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922
Shinokubo, Hiroshi	C-5080-2009	0000-0002-5321-2205
Fujii, Shintaro		0000-0003-2869-7674

ISSN: 2041-1723

Record 65 of 491

Title: Transverse Kerr effect in magnetic (Ga, Mn)As-based semiconductors and its applicability in waveguide isolators

Author(s): Wagenknecht, D (Wagenknecht, D.); Schmoranzerova, E (Schmoranzerova, E.); Trojanek, F (Trojanek, F.); Nemec, P (Nemec, P.); Ostatnicky, T (Ostatnicky, T.)

Source: JOURNAL OF APPLIED PHYSICS **Volume:** 122 **Issue:** 2 **Article Number:** 023104 **DOI:** 10.1063/1.4992126 **Published:** JUL 14 2017

Abstract: We report on the measurement of transverse Kerr effect in a diluted magnetic semiconductor Ga1-xMnxAs in visible and near infra-red spectral ranges. The relative change of reflectivity upon the change of the magnetization orientation is as large as 2%, the same order of magnitude as the response of ferromagnetic metals in the visible light. The experimental data are modeled by theoretical calculations, showing a very good match between the theory and the experiment. We further use the theoretical model in order to predict nonreciprocal losses in a planar waveguide. The predicted nonreciprocal losses are an order of magnitude larger as compared to devices with a Co/Fe ferromagnetic layer reported so far. Published by AIP Publishing.

Accession Number: WOS:000405663800005

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Wagenknecht, David	P-4165-2017	0000-0003-1927-9702
Nemec, Petr		0000-0001-6867-5942

ISSN: 0021-8979
eISSN: 1089-7550

Record 66 of 491

Title: WatAA: Atlas of Protein Hydration. Exploring synergies between data mining and ab initio calculations
Author(s): Cerny, J (Cerny, Jiri); Schneider, B (Schneider, Bohdan); Biedermannova, L (Biedermannova, Lada)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 26 **Pages:** 17094-17102 **DOI:** 10.1039/c7cp00187h **Published:** JUL 14 2017
Abstract: Water molecules represent an integral part of proteins and a key determinant of protein structure, dynamics and function. WatAA is a newly developed, web-based atlas of amino-acid hydration in proteins. The atlas provides information about the ordered first hydration shell of the most populated amino-acid conformers in proteins. The data presented in the atlas are drawn from two sources: experimental data and ab initio quantum-mechanics calculations. The experimental part is based on a data-mining study of a large set of high-resolution protein crystal structures. The crystal-derived data include 3D maps of water distribution around amino-acids and probability of occurrence of each of the identified hydration sites. The quantum mechanics calculations validate and extend this primary description by optimizing the water position for each hydration site, by providing hydrogen atom positions and by quantifying the interaction energy that stabilizes the water molecule at the particular hydration site position. The calculations show that the majority of experimentally derived hydration sites are positioned near local energy minima for water, and the calculated interaction energies help to assess the preference of water for the individual hydration sites. We propose that the atlas can be used to validate water placement in electron density maps in crystallographic refinement, to locate water molecules mediating protein-ligand interactions in drug design, and to prepare and evaluate molecular dynamics simulations.
Accession Number: WOS:000405422900016
PubMed ID: 28636001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cerny, Jiri	I-4733-2012	0000-0002-1969-9304
Schneider, Bohdan	D-2565-2009	0000-0001-7855-3690

ISSN: 1463-9076
eISSN: 1463-9084

Record 67 of 491

Title: Methane adsorption in ADOR zeolites: a combined experimental and DFT/CC study
Author(s): Rubes, M (Rubes, M.); Trachta, M (Trachta, M.); Koudelkova, E (Koudelkova, E.); Bulanek, R (Bulanek, R.); Kasneryk, V (Kasneryk, V.); Bludsky, O (Bludsky, O.)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 25 **Pages:** 16533-16540 **DOI:** 10.1039/c7cp02315d **Published:** JUL 7 2017
Abstract: Physical adsorption of methane in purely siliceous molecular sieves prepared by a recently discovered synthetic pathway using 2D zeolites as nanoscale building blocks has been investigated by means of combined experimental and theoretical approaches. The DFT/CC-based method has been tested on ADOR zeolites of the UTL family and a few experimentally well-characterized siliceous zeolites. Excellent agreement between theoretical and experimental heats of adsorption has been found for OKO, PCR, MFI, CHA and AEI zeolites. The observed discrepancy for the UTL germanosilicate (2 kJ mol(-1)) has been plausibly explained using a simple model of D4R defects. The proposed methodology can be used as a reliable characterization tool for newly synthesized silica nanomaterials.
Accession Number: WOS:000404530600026
PubMed ID: 28612872
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Trachta, Michal	G-8118-2014	0000-0001-5084-3434

ISSN: 1463-9076
eISSN: 1463-9084

Record 68 of 491

Title: Amino Acid Interaction (INTAA) web server
Author(s): Galgonek, J (Galgonek, Jakub); Vymetal, J (Vymetal, Jiri); Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri)
Source: NUCLEIC ACIDS RESEARCH **Volume:** 45 **Issue:** W1 **Pages:** W388-W392 **DOI:** 10.1093/nar/gkx352 **Published:** JUL 3 2017
Abstract: Large biomolecules-proteins and nucleic acids-are composed of building blocks which define their identity, properties and binding capabilities. In order to shed light on the energetic side of interactions of amino acids between themselves and with deoxyribonucleotides, we present the Amino Acid Interaction web server (http://bioinfo.uochb.cas.cz /INTAA/). INTAA offers the calculation of the residue Interaction Energy Matrix for any protein structure (deposited in Protein Data Bank or submitted by the user) and a comprehensive analysis of the interfaces in protein-DNA complexes. The Interaction Energy Matrix web application aims to identify key residues within protein structures which contribute significantly to the stability of the protein. The application provides an interactive user interface enhanced by 3D structure viewer for efficient visualization of pairwise and net interaction energies of individual amino acids, side chains and backbones. The protein-DNA interaction analysis part of the web server allows the user to view the relative abundance of various configurations of amino acid-deoxyribonucleotide pairs found at the protein-DNA interface and the interaction energies corresponding to these configurations calculated using a molecular mechanical force field. The effects of the sugar-phosphate moiety and of the dielectric properties of the solvent on the interaction energies can be studied for the various configurations.
Accession Number: WOS:000404427000058
PubMed ID: 28472475
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Jakubec, David	O-7570-2017	0000-0003-4288-0344
Vymetal, Jiri	R-1167-2017	0000-0002-0165-8707

ISSN: 0305-1048
eISSN: 1362-4962

Record 69 of 491

Title: Physical Map of the Short Arm of Bread Wheat Chromosome 3D
Author(s): Holusova, K (Holusova, Katerina); Vrana, J (Vrana, Jan); Safar, J (Safar, Jan); Simkova, H (Simkova, Hana); Balcarkova, B (Balcarkova, Barbora); Frenkel, Z (Frenkel, Zeev); Darrier, B (Darrier, Benoit); Paux, E (Paux, Etienne); Cattonaro, F (Cattonaro, Federica); Berges, H (Berges, Helene); Letellier, T (Letellier, Thomas); Alaux, M (Alaux, Michael); Dolezel, J (Dolezel, Jaroslav); Bartos, J (Bartos, Jan)
Source: PLANT GENOME **Volume:** 10 **Issue:** 2 **DOI:** 10.3835/plantgenome2017.03.0021 **Published:** JUL 2017
Abstract: Bread wheat (Triticum aestivum L.) is one of the most important crops worldwide. Although a reference genome sequence would represent a valuable resource for wheat improvement through genomics-assisted breeding and gene cloning, its generation has long been hampered by its allohexaploidy, high repeat content, and large size. As a part of a project coordinated by the International Wheat Genome Sequencing Consortium (IWGSC), a physical map of the short arm of wheat chromosome 3D (3DS) was prepared to facilitate reference genome assembly and positional gene cloning. It comprises 869 contigs with a cumulative length of 274.5 Mbp and represents 85.5% of the estimated chromosome arm size. Eighty-six Mbp of survey sequences from chromosome arm 3DS were assigned in silico to physical map contigs via next-generation sequencing of bacterial artificial chromosome pools, thus providing a high-density framework for physical map ordering along the chromosome arm. About 60% of the physical map was anchored in this single experiment. Finally, 1393 high-confidence genes were anchored to the physical map. Comparisons of gene space of the chromosome arm 3DS with genomes of closely related species [Brachypodium distachyon (L.) P. Beauv., rice (Oryza sativa L.), and sorghum [Sorghum bicolor (L.) Moench] and homeologous wheat chromosomes provided information about gene movement on the chromosome arm.
Accession Number: WOS:000410819500025

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bartos, Jan	F-6071-2014	
Frenkel, Zeev		0000-0003-0211-6966

ISSN: 1940-3372

Record 70 of 491

Title: Study on electronic properties, thermodynamic and kinetic parameters of the selected platinum(II) derivatives interacting with guanine

Author(s): Sebesta, F (Sebesta, Filip); Burda, JV (Burda, Jaroslav V.)

Source: JOURNAL OF INORGANIC BIOCHEMISTRY **Volume:** 172 **Pages:** 100-109 **DOI:** 10.1016/j.jinorgbio.2017.04.006 **Published:** JUL 2017

Abstract: Interaction of hydrated forms of several potential anticancer agents (PtCl2(diaminocyclohexane), trans-[PtCl2(NH3)(thiazole)], cis-[PtCl2(NH3)(piperidine)), and cis-PtCl2(NH3)(cyclohexylamine) complexes) with guanine are explored and compared with an analogous interaction of cisplatin. Basic electronic properties, binding and stabilization energies are determined and energy profiles for the aquation reaction are estimated at the B3LYP/6-311 + +G(2df,2pd) level of theory. It is found that the substitution reaction is art exothermic and exergonic process with Delta G slightly less negative than - 20 kcal/mol. The largest energy release occurs for PtCl(H2O)(diaminocyclohexane) complex. The rate constants for the Pt(II) complexes in the chloro- and hydroxoform are compared and an impact of the ligand in the trans position to water is discussed.

Accession Number: WOS:000404000300012

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
bUrda, Jaroslav		0000-0001-9909-8797

ISSN: 0162-0134

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Record 71 of 491

Title: A microscopic multiphonon approach to even and odd nuclei

Author(s): De Gregorio, G (De Gregorio, G.); Knapp, F (Knapp, F.); Lo Iudice, N (Lo Iudice, N.); Vesely, P (Vesely, P.)

Source: PHYSICA SCRIPTA **Volume:** 92 **Issue:** 7 **Article Number:** 074003 **DOI:** 10.1088/1402-4896/aa6fa2 **Published:** JUL 2017

Abstract: The formalism of an equation of motion phonon method is briefly outlined. In even-even nuclei, the method derives equations of motion which generate an orthonormal basis of correlated n-phonon states (n = 0, 1, 2,...), built of constituent Tamm-Dancoff phonons, and, then, solves the nuclear eigenvalue problem in such a multiphonon basis. In odd nuclei, analogous equations yield a basis of correlated orthonormal multiphonon particle-core states to be used for the solution of the full eigenvalue equations. The formalism does not rely on approximations, but lends itself naturally to simplifying assumptions. As illustrated here, the method has been implemented numerically for studying the electric dipole response in the heavy neutron rich Pb-208 and Sn-132 and in the odd O-17 and F-17. Self-consistent calculations, using a chiral inspired Hamiltonian, have confirmed the important role of the multiphonon states in enhancing the fragmentation of the strength in the giant and pygmy resonance regions consistently with the experimental data.

Accession Number: WOS:000403349800003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290
De Gregorio, Giovanni		0000-0003-0253-915X

ISSN: 0031-8949

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Record 72 of 491

Title: Crack bridging modelling in Bioglass (R) based scaffolds reinforced by poly-vinyl alcohol/microfibrillated cellulose composite coating

Author(s): Kotoul, M (Kotoul, Michal); Skalka, P (Skalka, Petr); Sevecek, O (Sevecek, Oldrich); Bertolla, L (Bertolla, Luca); Mertens, J (Mertens, James); Marcian, P (Marcian, Petr); Chawla, N (Chawla, Nikhilesh)

Source: MECHANICS OF MATERIALS **Volume:** 110 **Pages:** 16-28 **DOI:** 10.1016/j.mechmat.2017.04.004 **Published:** JUL 2017

Abstract: The paper deals with crack bridging modelling in Bioglass((R)) based scaffolds due the presence of a special polymer coating. This includes a careful modelling of the scaffold which is based on x-ray computed micro-tomography (micro-CT) scans and identification of bridging mechanism with the aid of extensive fractographic observations of coated, broken struts. A replacement of the real structure of scaffold by a periodic model utilizing Kelvin cell whose size corresponds to the mean cell size of the real foam is discussed. The struts of the idealized foam are modelled using the beam elements. A detailed computational analysis of crack bridging due to coating film fibrils under plane strain conditions is presented and an improvement of fracture resistance of coated scaffolds is explained. (c) 2017 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000402353000002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Skalka, Petr	G-9615-2014	0000-0002-7863-3372
Sevecek, Oldrich	F-8238-2013	0000-0003-3442-2650
Marcian, Petr		0000-0002-9458-9690

ISSN: 0167-6636

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Record 73 of 491

Title: Monte Carlo simulations of measured electron energy-loss spectra of diamond and graphite: Role of dielectric-response models

Author(s): Azzolini, M (Azzolini, Martina); Morresi, T (Morresi, Tommaso); Garberoglio, G (Garberoglio, Giovanni); Calliari, L (Calliari, Lucia); Pugno, NM (Pugno, Nicola M.); Taioli, S (Taioli, Simone); Dapor, M (Dapor, Maurizio)

Source: CARBON **Volume:** 118 **Pages:** 299-309 **DOI:** 10.1016/j.carbon.2017.03.041 **Published:** JUL 2017

Abstract: In this work we compare Monte Carlo (MC) simulations of electron-transport properties with reflection electron energy-loss measurements in diamond and graphite films. We assess the impact of different approximations of the dielectric response on the observables of interest for the characterization of carbon-based materials. We calculate the frequency-dependent dielectric response and energy-loss functions of these materials in two ways: a full ab initio approach, in which we carry out time-dependent density functional simulations in linear response for different momentum transfers, and a semi-classical model, based on the Drude-Lorentz extension to finite momenta of the optical dielectric function. Ab initio calculated dielectric functions lead to better agreement with measured energy-loss spectra compared to the widely used Drude-Lorentz model. This discrepancy is particularly evident for insulators and semiconductors beyond the optical limit (q not equal 0), where single-particle excitations become relevant. Furthermore, we show that the behaviour of the energy-loss function obtained at different accuracy levels has a dramatic effect on other physical observables, such as the inelastic mean free path and the stopping power in the low energy (<100 eV) regime and thus on the accuracy of MC simulations. (C) 2017 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000401120800035

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Taioli, Simone		0000-0003-4010-8000
Garberoglio, Giovanni		0000-0002-9201-2716

ISSN: 0008-6223

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Record 74 of 491

Title: Force field for realistic molecular dynamics simulations of TiO2 growth

Author(s): Houska, J (Houska, Jiri)

Source: COMPUTATIONAL MATERIALS SCIENCE **Volume:** 134 **Pages:** 1-7 **DOI:** 10.1016/j.commatsci.2017.03.024 **Published:** JUN 15 2017

Abstract: The paper deals with the development and subsequent testing of a Buckingham interaction potential which allows one to correctly describe the atom-by-atom growth of TiO2. Contrary to the most frequent procedures of the interaction potential development, correct coordination numbers which the potential leads to in an open surface growth are included amongst the criteria of success. First, parameters describing the short-range interaction have been fitted in order to achieve correct lattice parameters and formation energies in a wide range of Ti and O elemental charges. Next, growth simulations of amorphous TiO2 have been performed in order to investigate and quantify the relationship between the elemental charges and the preferred coordination numbers. The interaction potential which leads to the most experimentally relevant structures (in terms of coordination numbers) has been identified. This potential was further tested by growth simulations of crystalline TiO2. (C) 2017 Published by Elsevier B.V.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houska, Jiri	B-9616-2016	0000-0002-4809-4128

ISSN: 0927-0256

eISSN: 1879-0801

Record 75 of 491

Title: Relationships between the distribution of O atoms on partially oxidized metal (Al, Ag, Cu, Ti, Zr, Hf) surfaces and the adsorption energy: A density-functional theory study

Author(s): Houska, J (Houska, J.); Kozak, T (Kozak, T.)

Source: JOURNAL OF APPLIED PHYSICS **Volume:** 121 **Issue:** 22 **Article Number:** 225303 **DOI:** 10.1063/1.4985281 **Published:** JUN 14 2017

Abstract: We investigate the oxidation of selected metal (Al, Ag, Cu, Ti, Zr, and Hf) surfaces by the density functional theory. We go through a wide range of (233 per metal) distributions of O atoms on a partially oxidized metal surface. First, we focus on the qualitative information whether the preferred distribution of O atoms is heterogeneous (stoichiometric oxide + metal) or homogeneous (substoichiometric oxide). We find that the former is energetically preferred, e.g., for Al, while the latter is energetically preferred, e.g., for Ti, Zr, and Hf. Second, we provide the quantitative values of adsorption energies corresponding to the energetically preferred O atom distributions for various partial coverages of various metals by O. Third, we discuss and show an example of implications of the aforementioned findings for the understanding and simulations of sputtering. Published by AIP Publishing.

Accession Number: WOS:000403291200038

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houska, Jiri	B-9616-2016	0000-0002-4809-4128
Kozak, Tomas	A-9640-2016	0000-0002-5046-7253

ISSN: 0021-8979

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Record 76 of 491

Title: Magnetic character of holmium atom adsorbed on platinum surface

Author(s): Shick, AB (Shick, A. B.); Shapiro, DS (Shapiro, D. S.); Kolorenc, J (Kolorenc, J.); Lichtenstein, AI (Lichtenstein, A. I.)

Source: SCIENTIFIC REPORTS **Volume:** 7 **Article Number:** 2751 **DOI:** 10.1038/s41598-017-02809-7 **Published:** JUN 5 2017

Abstract: We address a recent controversy concerning the magnetic state of holmium adatom on platinum surface. Within a combination of the density functional theory (DFT) with the exact diagonalization (ED) of Anderson impurity model, the < J(Z)>=0 paramagnetic ground state | J= 8, J(z)=+/- 8> is found. In an external magnetic field, this state is transformed to a spin-polarized state with < J(z)>approximate to 6.7. We emphasize the role of 5d-4f interorbital exchange polarization in modification of the 4f shell energy spectrum.

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PubMed ID: 28584228

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Shick, Alexander	C-1420-2013	0000-0003-2700-5517
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302

ISSN: 2045-2322

Record 77 of 491

Title: Novel Tacrine-Scutellarin Hybrids as Multipotent Anti-Alzheimer's Agents: Design, Synthesis and Biological Evaluation

Author(s): Spilovska, K (Spilovska, Katarina); Korabecny, J (Korabecny, Jan); Sepsova, V (Sepsova, Vendula); Jun, D (Jun, Daniel); Hrabinova, M (Hrabinova, Martina); Jost, P (Jost, Petr); Muckova, L (Muckova, Lubica); Soukup, O (Soukup, Ondrej); Janockova, J (Janockova, Jana); Kucera, T (Kucera, Tomas); Dolezal, R (Dolezal, Rafael); Mezeiova, E (Mezeiova, Eva); Kaping, D (Kaping, Daniel); Kuca, K (Kuca, Kamil)

Source: MOLECULES **Volume:** 22 **Issue:** 6 **Article Number:** 1006 **DOI:** 10.3390/molecules22061006 **Published:** JUN 2017

Abstract: A novel series of 6-chlorotacrine-scutellarin hybrids was designed, synthesized and the biological activity as potential anti-Alzheimer's agents was assessed. Their inhibitory activity towards human acetylcholinesterase (hAChE) and human butyrylcholinesterase (hBChE), antioxidant activity, ability to cross the blood-brain barrier (BBB) and hepatotoxic profile were evaluated in vitro. Among these compounds, hybrid K1383, bearing two methylene tether between two basic scaffolds, was found to be very potent hAChE inhibitor (IC50 = 1.63 nM). Unfortunately, none of the hybrids displayed any antioxidant activity (EC50 500 M). Preliminary data also suggests a comparable hepatotoxic profile with 6-Cl-THA (established on a HepG2 cell line). Kinetic studies performed on hAChE with the most active compound in the study, K1383, pointed out to a mixed, non-competitive enzyme inhibition. These findings were further corroborated by docking studies.

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PubMed ID: 28621747

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Jun, Daniel	S-8647-2017	0000-0002-0882-6304
Kuca, Kamil		0000-0001-9664-1109
Hrabinova, Martina		0000-0002-9428-4109
Janockova, Jana		0000-0002-2034-1860
Spilovska, Katarina		0000-0003-3838-9149

ISSN: 1420-3049

Record 78 of 491

Title: Temporal profile of betatron radiation from laser-driven electron accelerators

Author(s): Horny, V (Horny, Vojtech); Nejdl, J (Nejdl, Jaroslav); Kozlova, M (Kozlova, Michaele); Krus, M (Krus, Miroslav); Bohacek, K (Bohacek, Karel); Petrzilka, V (Petrzilka, Vaclav); Klimo, O (Klimo, Ondrej)

Source: PHYSICS OF PLASMAS **Volume:** 24 **Issue:** 6 **Article Number:** 063107 **DOI:** 10.1063/1.4985687 **Published:** JUN 2017

Abstract: The temporal profile of X-ray betatron radiation was theoretically studied for the parameters available with current laser systems. Characteristics of the betatron radiation were investigated for three different configurations of laser wakefield acceleration: typical self-injection regime and optical injection regime with perpendicularly crossed injection and drive beams, both achievable with 100 TW class laser, and ionization injection regime with a sub-10 TW laser system that was experimentally verified. Constructed spectrograms demonstrate that X-ray pulse durations are in the order of few tens of femtoseconds and the optical injection case reveals the possibility of generating X-ray pulses as short as 2.6 fs.

The X-ray pulse duration depends mainly on the length of the trapped electron bunch as the emitted photons copropagate with the bunch with nearly the same velocity. These spectrograms were calculated using a novel simplified method based on the theory of Lienard-Wiechert potentials. It takes advantage of the fact that the electron oscillates transversally in the accelerating plasma wave in the wiggler regime and, thus, emits radiation almost exclusively in the turning points of its sine-like trajectory. Therefore, there are only few very narrow time intervals, which contribute significantly to the emission of radiation, while the rest can be neglected. These narrow time intervals are determined from the electron trajectories calculated using particle-in-cell simulations and the power spectrum at given point in far field is computed for each electron using the Fourier transform. Spectrograms of the emitted radiation are constructed by summing contributions of individual particles, since the incoherent nature of the electron bunch is assumed. Published by AIP Publishing.

Accession Number: WOS:000404639000065

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Klimo, Ondrej		0000-0002-0565-2409
Bohacek, Karel		0000-0001-6364-0599
Horny, Vojtech		0000-0002-4510-3770

ISSN: 1070-664X

eISSN: 1089-7674

Record 79 of 491

Title: Study of "source sheath" problem in PIC/MC simulation: Spherical geometry

Author(s): Trunec, D (Trunec, David); Zikan, P (Zikan, Petr); Wagner, J (Wagner, Jakub); Bonaventura, Z (Bonaventura, Zdenek)

Source: PHYSICS OF PLASMAS **Volume:** 24 **Issue:** 6 **Article Number:** 063508 **DOI:** 10.1063/1.4984990 **Published:** JUN 2017

Abstract: A method for treatment of boundary conditions and particle loading in a self-consistent semi-infinite Particle-In-Cell/Monte Carlo simulation is presented. A non-ionizing, collisional plasma in contact with an electrode was assumed. The simulation was performed for a spherical probe with constant probe potential. The motion of charged particles was calculated in three dimensions, but only the radial charge distribution and thus only radial electric field were assumed. The particle loading has to be done with an appropriate velocity distribution with a radial drift velocity. This drift velocity has to be calculated from the probe current, and therefore, a self-consistent (iterative) approach is necessary. Furthermore, correct values of particle densities and electric field potential at the outer boundary of the computational domain have to be set using asymptotic formulae for particle density and electric field potential. This approach removes the "source sheath" which is created artificially, if incorrect boundary conditions and velocity distributions of loaded particles are used. This approach is, however, feasible only for the case of a negative probe where asymptotic formulae are known. Published by AIP Publishing.

Accession Number: WOS:000404639000083

ISSN: 1070-664X

eISSN: 1089-7674

Record 80 of 491

Title: Repetitive DNA: A Versatile Tool for Karyotyping in Festuca pratensis Huds

Author(s): Krivankova, A (Krivankova, Anna); Kopecky, D (Kopecky, David); Stoces, S (Stoces, Stepan); Dolezel, J (Dolezel, Jaroslav); Hribova, E (Hribova, Eva)

Source: CYTOGENETIC AND GENOME RESEARCH **Volume:** 151 **Issue:** 2 **Pages:** 96-105 **DOI:** 10.1159/000462915 **Published:** JUN 2017

Abstract: FISH is a useful method to identify individual chromosomes in a karyotype and to discover their structural changes accompanying genome evolution and speciation. DNA probes for FISH should be chromosome specific and/or exhibit specific patterns of distribution along each chromosome. Such probes are not available in many plants including meadow fescue (Festuca pratensis Huds.), an important forage grass species. In the present study, various DNA repeats identified in Illumina shotgun sequences specific to chromosome 4F of F. pratensis were used as probes for FISH to develop the molecular karyotype of meadow fescue and to reveal a long-range molecular organization of its chromosomes. Five tandem repeats produced specific patterns on individual chromosomes. Their use in combination with probes for rRNA genes enabled the establishment of the molecular karyotype of meadow fescue. Most of the mobile genetic elements were dispersed along all the chromosomes except for the DNA transposon CACTA, which was localized preferentially to telomeric and subtelomeric regions, and a putative LTR element, which was localized to (peri) centromeric regions. Cytogenetic mapping of the 5 tandem repeats in other accessions of meadow fescue showed a highly similar distribution and confirmed the versatility and robustness of these probes. (C) 2017 S. Karger AG, Basel

Accession Number: WOS:000404007600005

PubMed ID: 28334706

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dolezel, Jaroslav	B-7716-2008	0000-0002-6263-0492

ISSN: 1424-8581

eISSN: 1424-859X

Record 81 of 491

Title: Exploring the Dynamics of Propeller Loops in Human Telomeric DNA Quadruplexes Using Atomistic Simulations

Author(s): Islam, B (Islam, Barira); Stadlbauer, P (Stadlbauer, Petr); Gil-Ley, A (Gil-Ley, Alejandro); Perez-Hernandez, G (Perez-Hernandez, Guillermo); Haider, S (Haider, Shozeb); Neidle, S (Neidle, Stephen); Bussi, G (Bussi, Giovanni); Banas, P (Banas, Pavel); Otyepka, M (Otyepka, Michal); Sponer, J (Sponer, Jiri)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 13 **Issue:** 6 **Pages:** 2458-2480 **DOI:** 10.1021/acs.jctc.7b00226 **Published:** JUN 2017

Abstract: We have carried out a series of extended unbiased molecular dynamics (MD) simulations (up to 10 its long, similar to 162 mu s in total) complemented by replica-exchange with the collective variable tempering (RECT) approach for several human telomeric DNA G-quadruplex (GQ) topologies with TTA propeller loops. We used different AMBER DNA force-field variants and also processed simulations by Markov State Model (MSM) analysis. The slow conformational transitions in the propeller loops took place on a scale of a few,us, emphasizing the need for long simulations in studies of GQ dynamics. The propeller loops sampled similar ensembles for all GQtopologies and for all force field dihedral-potential variants. The outcomes of standard and RECT simulations were consistent and captured similar spectrum of loop conformations. However, the most common crystallographic loop conformation was very unstable with all force-field versions. Although the loss of canonical gamma-trans state of the first propeller loop nucleotide could be related to the indispensable bsc0 alpha/gamma dihedral potential, even supporting this particular dihedral by a bias was insufficient to populate the experimentally dominant loop conformation. In conclusion, while our simulations were capable of providing a reasonable albeit not converged sampling of the TTA propeller loop conformational space, the force-field description still remained far from satisfactory.

Accession Number: WOS:000403530100010

PubMed ID: 28475322

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bussi, Giovanni	A-1776-2009	0000-0001-9216-5782
Otyepka, Michal		0000-0002-1066-5677

ISSN: 1549-9618

eISSN: 1549-9626

Record 82 of 491

Title: Exploring the Molecular-Level Architecture of the Active Compounds in Liquisolid Drug Delivery Systems Based on Mesoporous Silica Particles: Old Tricks for New Challenges

Author(s): Brus, J (Brus, Jiri); Albrecht, W (Albrecht, Wolfgang); Lehmann, F (Lehmann, Frank); Geier, J (Geier, Jens); Czernek, J (Czernek, Jiri); Urbanova, M (Urbanova, Martina); Kobera, L (Kobera, Libor); Jegorov, A (Jegorov, Alexand)

Source: MOLECULAR PHARMACEUTICS **Volume:** 14 **Issue:** 6 **Pages:** 2070-2078 **DOI:** 10.1021/acs.molpharmaceut.7b00167 **Published:** JUN 2017

Abstract: A general, easy-to-implement strategy for mapping the structure of organic phases integrated in mesoporous silica drug delivery devices is presented. The approach based on a few straightforward solid-state NMR techniques has no limitations regarding concentrations of the active compounds and enables straightforward discrimination of various organic phases. This way, among a range of typical arrangements of the active compounds and solvent molecules, a unique, previously unknown organogel phase of the self assembled tapentadol in glucofurol as a solvent was unveiled and clearly identified. Subsequently, with an aid of 2D H-1-H-1 MAS NMR and high-level quantum-chemical

calculations this uncommon low-molecular-weight organogel phase, existing exclusively in the porous system of the silica carrier, was described in detail. The optimized model revealed the tendency of tapentadol molecules to form hydrophobic arrangements through -OH center dot center dot center dot pi interactions combined with pi-pi stacking occurring in the core of API aggregates, thus precluding the formation of hydrogen bonds with the solvent. Overall, the proposed experimental approach allows for clear discrimination of a variety of local structures of active compounds loaded in mesoporous silica drug delivery devices in reasonably short time being applicable for advancement of novel drug delivery systems in pharmaceutical industry.

Accession Number: WOS:000402950500022

PubMed ID: 28485970

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Urbanova, Martina	G-9793-2014	0000-0003-1316-6395
Brus, Jiri	G-3459-2014	
Czernek, Jiri	H-6708-2014	
Kobera, Libor	G-5237-2014	0000-0002-8826-948X

ISSN: 1543-8384

Record 83 of 491

Title: Peculiarity of self-assembled cubic nanolamellae in the TiN/AlN system: Epitaxial self-stabilization by element deficiency/excess

Author(s): Zalesak, J (Zalesak, J.); Holec, D (Holec, D.); Matko, I (Matko, I.); Petrenec, M (Petrenec, M.); Sartory, B (Sartory, B.); Koutna, N (Koutna, N.); Daniel, R (Daniel, R.); Pitonak, R (Pitonak, R.); Keckes, J (Keckes, J.)

Source: ACTA MATERIALIA **Volume:** 131 **Pages:** 391-399 **DOI:** 10.1016/j.actamat.2017.04.009 **Published:** JUN 1 2017

Abstract: Synthesis of self-assembled thin films with multi -layered microstructures and outstanding functional properties represents a challenging task. In this work, detailed microstructural and chemical analyses of a self -assembled similar to 3.8 tm thick cubic (c) (AlxTi1-x)(y)N1-y film grown by low pressure chemical vapour deposition on a Al2O3(0001) substrate is discussed. The film with an overall x fraction of similar to 0.8 consists of alternating non-stoichiometric cubic Al-rich and Ti-rich nanolamellae with thicknesses of similar to 11 and similar to 1.5 nm. X-ray diffraction, electron microscopy and electron energy loss spectroscopy indicate that the nanolamellae coherency is primarily a result of an N deficiency in Ti-rich nanolamellae and an N excess in nanolamellae, which induce a decrease and an increase in nanolamellae lattice parameters, compared to the lattice parameters of stoichiometric rock-salt c-TiN and c-AIN, respectively. Therefore the self-assembly allows a formation of c-(AlxTi1-x)(y)N1-y nanolamellae with Al atomic fraction x of 0.9 -1.0, which are stabilized by neighbouring Ti-rich nanolamellae as a result of cube-on-cube epitaxy. The effect of the lattice parameter self-adjustment in the coherent nanolamellae by element deficiency and excess is verified by ab initio calculations. The compositional and morphological matches of the nano lamellae interfaces at the grain boundaries, the terraced growth with tetrahedral surface morphology and unzipped facets as well as the uniform nanolamellae thickness across the film depth indicate that the nanolamellae are formed as a result of kinetically-controlled oscillating reactions during the film growth. The understanding of this fascinating self -assembled nanolamellar microstructure containing a metastable c-AlNy, which does not exist in a bulk form at ambient conditions, represents a milestone in thin film technology. (C) 2017 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Accession Number: WOS:000402343400036

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sartory, Bernhard	A-7431-2013	
Keckes, Jozef		0000-0003-4770-4331

ISSN: 1359-6454

eISSN: 1873-2453

Record 84 of 491

Title: Phomopsis longicolla RNA virus 1-Novel virus at the edge of myco- and plant viruses

Author(s): Hrabakova, L (Hrabakova, Lenka); Koloniuk, I (Koloniuk, Igor); Petrzik, K (Petrzik, Karel)

Source: VIROLOGY **Volume:** 506 **Pages:** 14-18 **DOI:** 10.1016/j.virol.2017.03.003 **Published:** JUN 2017

Abstract: The complete nucleotide sequence of a new RNA mycovirus in the KY isolate of Phomopsis longicolla Hobbs 1985 and its protoplasts subcultures p5, p9, and ME711 was discovered. The virus, provisionally named Phomopsis longicolla RNA virus 1 (PlRV1), was localized in mitochondria and was determined to have a genome 2822 nucleotides long. A single open reading frame could be translated in silico by both standard and mitochondrial genetic codes into a product featuring conservative domains for an RNA-dependent RNA polymerase (RdRp). The RdRp of PlRV1 has no counterpart among mycoviruses, but it is about 30% identical with the RdRp of plant ourmiaviruses. Recently, new mycoviruses related to plant ourmiaviruses and forming one Glade with PlRV1 have been discovered. This separate Glade could represent the crucial link between plant and fungal viruses.

Accession Number: WOS:000400416200003

PubMed ID: 28288321

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Petrzik, Karel	B-6957-2008	
Hrabakova, Lenka	H-2510-2015	
Koloniuk, Igor	G-9526-2014	0000-0002-5893-6683

ISSN: 0042-6822

Record 85 of 491

Title: Formation of planarized intramolecular charge-transfer state in dichlorotriazinyl-pyrene fluorescent probe: TD-DFT and resonance Raman study

Author(s): Stanek, T (Stanek, Tomas); Dvorak, M (Dvorak, Miroslav); Almonasy, N (Almonasy, Numan); Nepras, M (Nepras, Milos); Sloufova, I (Sloufova, Ivana); Michl, M (Michl, Martin)

Source: DYES AND PIGMENTS **Volume:** 141 **Pages:** 121-127 **DOI:** 10.1016/j.dyepig.2017.01.077 **Published:** JUN 2017

Abstract: This study is focused on explanation of the remarkable photophysical behaviour of the 1-(4,6-dichloro-1,3,5-triazin-2-yl)-pyrene (PyTC2) compound which has been introduced as a fluorescent polarity probe. This compound exhibits large solvatochromic red-shift of fluorescence emission band while maintaining high fluorescence quantum yield and monoexponential decay kinetics throughout the whole solvent polarity scale. As the semi-empirical calculations reported in the original paper have not revealed any excited state possessing a high dipole moment, it has been suggested that the red-shift originates from planarization of the emitting excited state in polar solvents in contrast to unchanged twisted geometry in non-polar solvents. However, both the extent of the red-shift and the disappearance of the vibronic structure in polar solvents indicate that the emission originates from an excited state with high dipole moment and that the semi-empirical methods may not be sufficient to describe the emitting state of this molecule correctly. Thus, we have performed TD-DFT calculations including the potential energy surface scans. According to these calculations and scans, the emission takes place from a planarized intramolecular charge-transfer (ICT) state. This is in good agreement with all aspects of the observed fluorescence behaviour of PyTC2. Independent experimental evidence for the ICT has been provided by analysis of resonance Raman intensities where bands corresponding to enhanced normal modes residing on triazine and the stretching mode between pyrene and triazine moieties have been identified. The formation of the photoinduced ICT together with easy and inexpensive preparation make this compound and its derivatives candidate as push-pull building blocks for the design of advanced functional materials. (C) 2017 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000399852700015

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sloufova, Ivana	F-5344-2014	0000-0002-4757-6029

ISSN: 0143-7208

eISSN: 1873-3743

Record 86 of 491

Title: Stable Au-C bonds to the substrate for fullerene-based nanostructures

Author(s): Chutora, T (Chutora, Taras); Redondo, J (Redondo, Jesus); de la Torre, B (de la Torre, Bruno); Svec, M (Svec, Martin); Jelinek, P (Jelinek, Pavel); Vazquez, H (Vazquez, Hector)

Source: BEILSTEIN JOURNAL OF NANOTECHNOLOGY **Volume:** 8 **Pages:** 1073-1079 **DOI:** 10.3762/bjnano.8.109 **Published:** MAY 17 2017

Abstract: We report on the formation of fullerene-derived nanostructures on Au(111) at room temperature and under UHV conditions. After low-energy ion sputtering of fullerene films deposited on Au(111), bright spots appear at the herringbone corner sites when measured using a scanning tunneling microscope. These features are stable at room temperature against diffusion on the surface. We carry out DFT calculations of fullerene molecules having one missing carbon atom to simulate the vacancies in the molecules resulting from the sputtering process. These modified fullerenes have an adsorption energy on the Au(111) surface that is 1.6 eV higher than that of C-60 molecules. This increased binding energy arises from the saturation by the Au surface of the bonds around the molecular vacancy defect. We therefore interpret the observed features as adsorbed fullerene-derived molecules with C vacancies. This provides a pathway for the formation of fullerene-based nanostructures on Au at room temperature.

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PubMed ID: 28685108

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Svec, Martin	G-6645-2014	
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922

ISSN: 2190-4286

Record 87 of 491

Title: Side Reactions with an Equilibrium Constraint: Detailed Mechanism of the Substitution Reaction of Tetraplatin with dGMP as a Starting Step of the Platinum(IV) Reduction Process

Author(s): Sebesta, F (Sebesta, Filip); Burda, JV (Burda, Jaroslav V.)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 121 **Issue:** 17 **Pages:** 4400-4413 **DOI:** 10.1021/acs.jpcb.7b01427 **Published:** MAY 4 2017

Abstract: Two possible pathways of the substitution reaction within the reduction process of the Pt-IV(DACH)Cl-4 by dGMP are compared: associative reaction course and autocatalytic Basolo-Pearson mechanisms. Since two forms: single-protonated and fully deprotonated phosphate group of dGMP are present in equilibrium at neutral and mildly acidic solutions, consideration of a side reactions scheme with acido-basic equilibrium-constraint is a very important model for obtaining reliable results. The examined complexes are optimized at the B3LYP-GD3BJ/6-31G(d)level with the COSMO implicit solvation model and Klamt's radii used for cavity construction. Energy characteristics and thermodynamics for all reaction branches are determined using the B3LYP-GD3BJ/6-311++G(2df,2pd)/IEF-PCM/scaled-UAKS level with Wertz's entropy corrections. Rate constants are estimated for each individual branch according to Eyring's transition state theory (TST), averaged according to equilibrium constraint and compared with available experimental data. The determined reaction barriers of the autocatalytic pathway fairly correspond with experimental values. Furthermore, autocatalytic reaction of tetraplatin and its two analogues complexes [Pt-IV(en)Cl-4 and Pt-IV(NH3)(2)Cl-4] are explored and compared with measured data in order to examined general reaction descriptors.

Accession Number: WOS:000400881300008

PubMed ID: 28394593

Author Identifiers:

Author	ResearcherID Number	ORCID Number
bUrda, Jaroslav		0000-0001-9909-8797

ISSN: 1520-6106

Record 88 of 491

Title: Exploring the optoelectronic properties of Nitrido-magneso-silicates: Ca[Mg3SiN4], Sr[Mg3SiN4], and Eu[Mg3SiN4]

Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Goumri-Said, S (Goumri-Said, Souraya)

Source: SEMICONDUCTOR SCIENCE AND TECHNOLOGY **Volume:** 32 **Issue:** 5 **Article Number:** 055017 **DOI:** 10.1088/1361-6641/aa62bd **Published:** MAY 2017

Abstract: Optoelectronic properties of the Nitrido-magneso-silicates Ca[Mg3SiN4], Sr[Mg3SiN4], and Eu[Mg3SiN4] compounds have been investigated using the relativistic full-potential augmented plane-wave method (FLAPW) based on the density functional theory (DFT). The calculations of the electronic and optical properties were conducted by using the local density approximation (LDA), generalized gradient approximation (GGA), and modified Becke Johnson (mBJ) potential. A study of the band structures shows that these compounds are indirect band gap materials. We found a great variation in the obtained energy band gap value as we changed the functionals. The mBJ functional leads to a greater band-gap value compared to LDA and GGA cases. Based on the calculated electronic structure, the optical properties computed, such as the complex dielectric function, absorption coefficient, reflectivity, energy loss function and refractive index, were functions of the photon energy. Origins of the spectral peaks in the optical spectra were discussed and assigned to different electronic transitions observed from the electronic structure calculation.

Accession Number: WOS:000413491400004

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Azam, Sikander		0000-0001-5923-1127

ISSN: 0268-1242

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Record 89 of 491

Title: Blind Deconvolution With Model Discrepancies

Author(s): Kotera, J (Kotera, Jan); Smidl, V (Smidl, Vaclav); Sroubek, F (Sroubek, Filip)

Source: IEEE TRANSACTIONS ON IMAGE PROCESSING **Volume:** 26 **Issue:** 5 **Pages:** 2533-2544 **DOI:** 10.1109/TIP.2017.2676981 **Published:** MAY 2017

Abstract: Blind deconvolution is a strongly ill-posed problem comprising of simultaneous blur and image estimation. Recent advances in prior modeling and/or inference methodology led to methods that started to perform reasonably well in real cases. However, as we show here, they tend to fail if the convolution model is violated even in a small part of the image. Methods based on variational Bayesian inference play a prominent role. In this paper, we use this inference in combination with the same prior for noise, image, and blur that belongs to the family of independent non-identical Gaussian distributions, known as the automatic relevance determination prior. We identify several important properties of this prior useful in blind deconvolution, namely, enforcing non-negativity of the blur kernel, favoring sharp images over blurred ones, and most importantly, handling non-Gaussian noise, which, as we demonstrate, is common in real scenarios. The presented method handles discrepancies in the convolution model, and thus extends applicability of blind deconvolution to real scenarios, such as photos blurred by camera motion and incorrect focus.

Accession Number: WOS:000399396400034

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Record 90 of 491

Title: Intercellular crosstalk in human malignant melanoma

Author(s): Dvorankova, B (Dvorankova, Barbora); Szabo, P (Szabo, Pavol); Kodet, O (Kodet, Ondrej); Strnad, H (Strnad, Hynek); Kolar, M (Kolar, Michal); Lacina, L (Lacina, Lukas); Krejci, E (Krejci, Eliska); Nanka, O (Nanka, Ondrej); Sedo, A (Sedo, Aleksi); Smetana, K (Smetana, Karel, Jr.)

Source: PROTOPLASMA **Volume:** 254 **Issue:** 3 **Special Issue:** SI **Pages:** 1143-1150 **DOI:** 10.1007/s00709-016-1038-z **Published:** MAY 2017

Abstract: Incidence of malignant melanoma is increasing globally. While the initial stages of tumors can be easily treated by a simple surgery, the therapy of advanced stages is rather limited. Melanoma cells spread rapidly through the body of a patient to form multiple metastases. Consequently, the survival rate is poor. Therefore, emphasis in melanoma research is given on early diagnosis and development of novel and more potent therapeutic options. The malignant melanoma is arising from melanocytes, cells protecting mitotically active keratinocytes against damage caused by UV light irradiation. The melanocytes originate in the neural crest and consequently migrate to the epidermis. The relationship between the melanoma cells, the melanocytes, and neural crest stem cells manifests when the melanoma cells are implanted to an early embryo: they use similar migratory routes as the normal neural crest cells. Moreover, malignant potential of these melanoma cells is overdriven in this experimental model, probably due to microenvironmental reprogramming. This observation demonstrates the crucial role of the microenvironment in melanoma biology. Indeed, malignant tumors in general represent complex ecosystems, where multiple cell

types influence the growth of genetically mutated cancer cells. This concept is directly applicable to the malignant melanoma. Our review article focuses on possible strategies to modify the intercellular crosstalk in melanoma that can be employed for therapeutic purposes.

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Conference Title: 12th International Congress of Cell Biology (ICCB)

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Conference Location: Prague, CZECH REPUBLIC

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Smetana, Karel	D-7039-2017	0000-0002-7878-8403
Szabo, Pavol	R-5197-2016	0000-0002-1944-1493
Dvorankova, Barbora	R-2316-2016	0000-0002-3914-9668
Kolar, Michal	A-3307-2012	0000-0002-4593-1525
Kodet, Ondrej	A-1267-2017	0000-0002-1382-2535
Krejci, Eliska	G-3034-2014	0000-0002-3394-9971
Lacina, Lukas		0000-0002-1750-9933
Nanka, Ondrej		0000-0002-6300-395X

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Record 91 of 491

Title: Steam Torch Plasma Modelling

Author(s): Jenista, J (Jenista, Jiri)

Source: PLASMA CHEMISTRY AND PLASMA PROCESSING **Volume:** 37 **Issue:** 3 **Special Issue:** SI **Pages:** 653-687 **DOI:** 10.1007/s11090-017-9789-7 **Published:** MAY 2017

Abstract: Numerical modelling of physical properties and processes in an electric arc stabilized by a water vortex (steam torch) has been summarized in this review paper. One-fluid MHD equations are numerically solved for an axisymmetric thermal plasma flow inside a discharge chamber of the steam plasma torch. The steady state solution results are discussed for the range of currents 300-600 A with relatively low steam flow rate of about 0.3 g s(-1). The maximum obtained velocities and temperatures-8500 m s(-1), 26,300 K, are reported at the centre of the nozzle exit for 600 A. The evaporation of water, i.e. mass flow rate of steam, was predicted from a comparison between the present simulation and experiments. The generated plasma is mildly compressible (M < 0.7) with the inertial forces overwhelming the magnetic, viscous, centrifugal and Coriolis forces with the factor of 10(3). Our calculations showed that the most significant processes determining properties of the arc are the balance of the Joule heat with radiation and radial conduction losses from the arc. Rotation of plasma column due to the tangential velocity component has a negligible effect on the overall arc performance, however, the rotation of water induces fluctuations in the arc and in the plasma jet with characteristic frequency which is related to the frequency of rotation of water. Reabsorption of radiation occurs at the radial position higher than 2.5 mm from the arc axis. The amount of reabsorbed radiation is between 17 and 28%. LTE conditions are satisfied in the arc column with the 2 mm radius. Comparison between the present simulations and experiments shows good agreement with the current-voltage characteristics, radial velocity and temperature profiles, as well as with the other related numerical simulation.

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Record 92 of 491

Title: Properties of the Only Thorium Fullerene, Th@C-84, Uncovered

Author(s): Kaminsky, J (Kaminsky, Jakub); Vicha, J (Vicha, Jan); Bour, P (Bour, Petr); Straka, M (Straka, Michal)

Source: JOURNAL OF PHYSICAL CHEMISTRY A **Volume:** 121 **Issue:** 16 **Pages:** 3128-3135 **DOI:** 10.1021/acs.jpca.7b00346 **Published:** APR 27 2017

Abstract: Only a single thorium fullerene, Th@C-84, has been reported to date (Akiyama, K.; et al. J. Nucl. Radiochem. Sci. 2002, 3, 151-154). Although the system was characterized by UV-vis and XANES (X-ray absorption near edge structure) spectra, its structure and properties remain unknown. In this work we used the density functional calculations to identify molecular and electronic structure of the Th@C-84. Series of molecular structures satisfying the ThC84 stoichiometric formula were studied comprising 24 IPR and 110 non-IPR Th@C-84 isomers as well as 9 ThC2@C-82 IPR isomers. The lowest energy structure is Th@C-84-C-s(10) with the singlet ground state. Its predicted electronic absorption spectra are in agreement with the experimentally observed ones. The bonding between the cage and Th was characterized as polar covalent with Th in formal oxidation state IV. The NMR chemical shifts of Th@C-84-C-s(10) were predicted to guide the future experimental efforts in identification of this compound.

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PubMed ID: 28375617

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vicha, Jan	D-8417-2012	0000-0003-3698-8236
Straka, Michal	E-5246-2011	0000-0002-7857-4990
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022

ISSN: 1089-5639

Record 93 of 491

Title: Relation between molecular electronic structure and nuclear spin-induced circular dichroism

Author(s): Stepanek, P (Stepanek, Petr); Coriani, S (Coriani, Sonia); Sundholm, D (Sundholm, Dage); Ovchinnikov, VA (Ovchinnikov, Vasily A.); Vaara, J (Vaara, Juha)

Source: SCIENTIFIC REPORTS **Volume:** 7 **Article Number:** 46617 **DOI:** 10.1038/srep46617 **Published:** APR 24 2017

Abstract: The recently theoretically described nuclear spin-induced circular dichroism (NSCD) is a promising method for the optical detection of nuclear magnetization. NSCD involves both optical excitations of the molecule and hyperfine interactions and, thus, it offers a means to realize a spectroscopy with spatially localized, high-resolution information. To survey the factors relating the molecular and electronic structure to the NSCD signal, we theoretically investigate NSCD of twenty structures of the four most common nucleic acid bases (adenine, guanine, thymine, cytosine). The NSCD signal correlates with the spatial distribution of the excited states and couplings between them, reflecting changes in molecular structure and conformation. This constitutes a marked difference to the nuclear magnetic resonance (NMR) chemical shift, which only reflects the local molecular structure in the ground electronic state. The calculated NSCD spectra are rationalized by means of changes in the electronic density and by a sum-over-states approach, which allows to identify the contributions of the individual excited states. Two separate contributions to NSCD are identified and their physical origins and relative magnitudes are discussed. The results underline NSCD spectroscopy as a plausible tool with a power for the identification of not only different molecules, but their specific structures as well.

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PubMed ID: 28436463

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Stepanek, Petr	G-7636-2014	0000-0001-5000-8180
Coriani, Sonia	B-6424-2011	0000-0002-4487-897X
Sundholm, Dage Matts Borje		0000-0002-2367-9277

ISSN: 2045-2322

Record 94 of 491

Title: Automated numerical calculation of Sagnac correction for photonic paths

Author(s): Slapak, M (Slapak, Martin); Vojtech, J (Vojtech, Josef); Velc, R (Velc, Radek)

Source: OPTICS COMMUNICATIONS **Volume:** 389 **Pages:** 230-233 **DOI:** 10.1016/j.optcom.2016.12.029 **Published:** APR 15 2017

Abstract: Relativistic effects must be taken into account for highly accurate time and frequency transfers. The most important is the Sagnac correction which is also source of non-reciprocity in various directions of any transfer in relation with the Earth rotation. In this case, not all important parameters as exact trajectory of the optical fibre path (leased fibres) are known with sufficient precision thus it is necessary to estimate lower and upper bounds of computed corrections. The presented approach deals with uncertainty in knowledge of detailed fibre paths, and also with complex paths with loops. We made the whole process of calculation of the Sagnac correction fully automated.

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ISSN: 0030-4018

eISSN: 1873-0310

Record 95 of 491

Title: Dubins Orienteering Problem

Author(s): Penicka, R (Penicka, Robert); Faigl, J (Faigl, Jan); Vana, P (Vana, Petr); Saska, M (Saska, Martin)

Source: IEEE ROBOTICS AND AUTOMATION LETTERS **Volume:** 2 **Issue:** 2 **Pages:** 1210-1217 **DOI:** 10.1109/LRA.2017.2666261 **Published:** APR 2017

Abstract: In this letter, we address the orienteering problem (OP) for curvature constrained vehicle. For a given set of target locations, each with associated reward, the OP stands to find a tour from a prescribed starting location to a given ending location such that it maximizes collected rewards while the tour length is within a given travel budget constraint. The addressed generalization of the EuclideanOP is called the Dubins Orienteering Problem (DOP) in which the reward collecting tour has to satisfy the limited turning radius of the Dubins vehicle. The DOP consists not only of selecting the most valuable targets and determination of the optimal sequence to visit them, but it also involves the determination of the vehicle's heading angle at each target location. The proposed solution is based on the Variable neighborhood search technique, and its feasibility is supported by an empirical evaluation in existing OP benchmarks. Moreover, an experimental verification in a real practical scenario further demonstrates the necessity of the proposed direct solution of the Dubins Orienteering Problem.

Accession Number: WOS:000413736600109

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vana, Petr	K-5165-2017	0000-0003-2155-5788

ISSN: 2377-3766

Record 96 of 491

Title: Route towards Dirac and Weyl antiferromagnetic spintronics

Author(s): Smejkal, L (Smejkal, Libor); Jungwirth, T (Jungwirth, Tomas); Sinova, J (Sinova, Jairo)

Source: PHYSICA STATUS SOLIDI-RAPID RESEARCH LETTERS **Volume:** 11 **Issue:** 4 **Special Issue:** SI **Article Number:** 1700044 **DOI:** 10.1002/pssr.201700044 **Published:** APR 2017

Abstract: Topological quantum matter and spintronics research have been developed to a large extent independently. In this review, we discuss a new role that the antiferromagnetic order has taken in combining topological matter and spintronics. This occurs due to the complex microscopic symmetries present in antiferromagnets that allow for, e.g., topological relativistic quasiparticles and the newly discovered Neel spin-orbit torques to coexist. We first introduce the concepts of topological semimetals and spin-orbitronics. Secondly, we explain the antiferromagnetic symmetries on a minimal Dirac semimetal model and the guiding role of ab initio calculations in predictions of examples of Dirac and Weyl antiferromagnets: SrMnBi2, CuMnAs, and Mn3Ge. Lastly, we illustrate the interplay of Dirac quasiparticles, topology and antiferromagnetism on: (i) the experimentally observed quantum Hall effect in EuMnBi2; (ii) the large anomalous Hall effect in Mn3Ge; and (iii) the theoretically predicted topological metal-insulator transition in CuMnAs. Dirac fermions at the Fermi level of the Dirac semimetal antiferromagnet calculated from the fist-principles. Reorientation of the Neel vector drives the topological metal-insulator transition. (C) 2017 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

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Record 97 of 491

Title: Atomistic Modeling-Based Design of Novel Materials

Author(s): Holec, D (Holec, David); Zhou, LC (Zhou, Liangcai); Riedl, H (Riedl, Helmut); Koller, CM (Koller, Christian M.); Mayrhofer, PH (Mayrhofer, Paul H.); Friak, M (Friak, Martin); Sob, M (Sob, Mojmir); Kormann, F (Kormann, Fritz); Neugebauer, J (Neugebauer, Joerg); Music, D (Music, Denis); Hartmann, MA (Hartmann, Markus A.); Fischer, FD (Fischer, Franz D.)

Source: ADVANCED ENGINEERING MATERIALS **Volume:** 19 **Issue:** 4 **Special Issue:** SI **Article Number:** UNSP 1600688 **DOI:** 10.1002/adem.201600688 **Published:** APR 2017

Abstract: Modern materials science increasingly advances via a knowledge-based development rather than a trial-and-error procedure. Gathering large amounts of data and getting deep understanding of non-trivial relationships between synthesis of materials, their structure and properties is experimentally a tedious work. Here, theoretical modeling plays a vital role. In this review paper we briefly introduce modeling approaches employed in materials science, their principles and fields of application. We then focus on atomistic modeling methods, mostly quantum mechanical ones but also Monte Carlo and classical molecular dynamics, to demonstrate their practical use on selected examples.

Accession Number: WOS:000399952600015

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Music, Denis	C-2978-2012	0000-0003-2303-3676
Kormann, Fritz	A-5677-2012	0000-0003-3050-6291
Hartmann, Markus	A-3567-2016	0000-0001-6046-0365
Riedl, Helmut		0000-0002-8108-1185
Mayrhofer, Paul		0000-0001-7328-9333

ISSN: 1438-1656

eISSN: 1527-2648

Record 98 of 491

Title: GvL effects in T-prolymphocytic leukemia: evidence from MRD kinetics and TCR repertoire analyses

Author(s): Sellner, L (Sellner, L.); Bruggemann, M (Brueggemann, M.); Schlitt, M (Schlitt, M.); Knecht, H (Knecht, H.); Herrmann, D (Herrmann, D.); Reigl, T (Reigl, T.); Krejci, A (Krejci, A.); Bystry, V (Bystry, V.); Darzentas, N (Darzentas, N.); Rieger, M (Rieger, M.); Dietrich, S (Dietrich, S.); Luft, T (Luft, T.); Ho, AD (Ho, A. D.); Kneba, M (Kneba, M.); Dreger, P (Dreger, P.)

Source: BONE MARROW TRANSPLANTATION **Volume:** 52 **Issue:** 4 **Pages:** 544-551 **DOI:** 10.1038/bmt.2016.305 **Published:** APR 2017

Abstract: Allogeneic stem cell transplantation (alloSCT) is used for treating patients with T-prolymphocytic leukemia (T-PLL). However, direct evidence of GvL activity in T-PLL is lacking. We correlated minimal residual disease (MRD) kinetics with immune interventions and T-cell receptor (TCR) repertoire diversity alterations in patients after alloSCT for T-PLL. Longitudinal quantitative MRD monitoring was performed by clone-specific real-time PCR of TCR rearrangements (n = 7), and TCR repertoire diversity assessment by nextgeneration sequencing (NGS; n = 3) Although post-transplant immunomodulation (immunosuppression tapering or donor lymphocyte infusions) resulted in significant reduction (>1 log) of MRD levels in 7 of 10 occasions, durable MRD clearance was observed in only two patients. In all three patients analyzed by TCR-NGS, MRD responses were reproducibly associated with a shift from a clonal, T-PLL-driven profile to a polyclonal signature. Novel clonotypes that could explain a clonal GvL effect did not emerge. In conclusion, TCR-based MRD quantification appears to be a suitable tool for monitoring and guiding treatment interventions in T-PLL. The MRD responses to immune modulation observed here provide first molecular evidence for GvL activity in T-PLL which, however, may be often only transient and reliant on a poly-/oligoclonal rather than a monoclonal T-cell response.

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PubMed ID: 27941777

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sellner, Leopold		0000-0002-7893-401X

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Record 99 of 491

Title: Argumentation Mining in User-Generated Web Discourse

Author(s): Habernal, I (Habernal, Ivan); Gurevych, I (Gurevych, Iryna)

Source: COMPUTATIONAL LINGUISTICS **Volume:** 43 **Issue:** 1 **Pages:** 125-179 **DOI:** 10.1162/COLI_a_00276 **Published:** APR 2017

Abstract: The goal of argumentation mining, an evolving research field in computational linguistics, is to design methods capable of analyzing people's argumentation. In this article, we go beyond the state of the art in several ways. (i) We deal with actual Web data and take up the challenges given by the variety of registers, multiple domains, and unrestricted noisy user-generated Web discourse. (ii) We bridge the gap between normative argumentation theories and argumentation phenomena encountered in actual data by adapting an argumentation model tested in an extensive annotation study. (iii) We create a new gold standard corpus (90k tokens in 340 documents) and experiment with several machine learning methods to identify argument components. We offer the data, source codes, and annotation guidelines to the community under free licenses. Our findings show that argumentation mining in user-generated Web discourse is a feasible but challenging task.

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ISSN: 0891-2017
eISSN: 1530-9312

Record 100 of 491

Title: Radiative association of He(2(3)P) with lithium cations: Pi -> Sigma processes

Author(s): Zamecnikova, M (Zamecnikova, Martina); Kraemer, WP (Kraemer, Wolfgang P.); Soldan, P (Soldan, Pavel)

Source: JOURNAL OF QUANTITATIVE SPECTROSCOPY & RADIATIVE TRANSFER **Volume:** 191 **Pages:** 88-95 **DOI:** 10.1016/j.jqsrt.2017.01.019 **Published:** APR 2017

Abstract: The radiative association processes originating in the 1(3)Pi continuum of the He (2(3)P)+ Li+ collisional system are investigated in this study. The calculations of the dynamic collision processes are based on highly accurate state-of-the-art ab initio calculations of the potential energy functions for the 1(3)Pi and the three lowest (3)Sigma states of HeLi+ and the associated transition dipole-moment functions. Cross-sections for the spontaneous and stimulated radiative association processes are calculated as functions of collision energy. The corresponding rate coefficients characterizing the efficiency of the formation of the molecular ion in its a(3)Sigma(+), b(3)Sigma(+), and c(3)Sigma(+) states from the initial 1(3)Pi state are obtained over a wide range of temperatures. At very low temperatures the 1 -> b process has a maximum rate-coefficient value of about 7.9 x 10(-13) cm(3) s(-1), whereas process 1 -> a reaches its maximum value of 2.0 x 10(-13) cm(3) s(-1) at a temperature of about 500 K. Altogether the three radiative association processes investigated here can be considered as the continuum-to-bound state radiative transition part of the total quenching of the initial collision channel. (C) 2017 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000398647600012

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zamecnikova, Martina	H-3552-2014	0000-0003-1619-3583
Soldan, Pavel	C-2256-2008	0000-0002-6281-7599

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Page 3 (Records 101 -- 150)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 101 of 491

Title: Reducing the dimensionality of grid based methods for electron-atom scattering calculations below ionization threshold

Author(s): Benda, J (Benda, Jakub); Houfek, K (Houfek, Karel)

Source: COMPUTER PHYSICS COMMUNICATIONS **Volume:** 213 **Pages:** 46-51 **DOI:** 10.1016/j.cpc.2016.12.001 **Published:** APR 2017

Abstract: For total energies below the ionization threshold it is possible to dramatically reduce the computational burden of the solution of the electron-atom scattering problem based on grid methods combined with the exterior complex scaling. As in the R-matrix method, the problem can be split into the inner and outer problem, where the outer problem considers only the energetically accessible asymptotic channels. The (N + 1)-electron inner problem is coupled to the one-electron outer problems for every channel, resulting in a matrix that scales only linearly with size of the outer grid. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000393630800006

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houfek, Karel	P-2300-2017	0000-0002-7974-0399
Benda, Jakub		0000-0003-0965-2040

ISSN: 0010-4655

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Record 102 of 491

Title: Chlorine intercalation in graphitic carbon nitride for efficient photocatalysis

Author(s): Liu, CY (Liu, Chengyin); Zhang, YH (Zhang, Yihe); Dong, F (Dong, Fan); Reshak, AH (Reshak, A. H.); Ye, LQ (Ye, Liqun); Pinna, N (Pinna, Nicola); Zeng, C (Zeng, Chao); Zhang, TR (Zhang, Tierui); Huang, HW (Huang, Hongwei)

Source: APPLIED CATALYSIS B-ENVIRONMENTAL **Volume:** 203 **Pages:** 465-474 **DOI:** 10.1016/j.apcatb.2016.10.002 **Published:** APR 2017

Abstract: Metal-free graphitic carbon nitride (g-C3N4) shows tremendous potentials in energy and environmental domains. Nonetheless, amelioration on the crystal configuration, electronic structure and microstructure of g-C3N4 for high-performing visible-light photocatalysis is still challenging and anticipated. Here we report the development of chlorine (Cl) intercalated g-C3N4 via co-pyrolysis of melamine and excessive ammonium chloride (excessive is very pivotal). This protocol renders not only Cl intercalation in the interlayer of g-C3N4, but also a homogeneous porous structure, thereby endowing g-C3N4 with multiple superiority effects, including significantly promoted charge migration by establishing interlayer pathway, up-shifted conduction-band level, narrowed band gap as well as enhanced surface area. The as-prepared CI intercalated mesoporous g-C3N4 parades outstanding photocatalytic performance for water splitting into H-2, CO2 reduction, liquid and air contaminants removal. The most enhanced photocatalytic performance was obtained at Cl-C3N4-3 for H-2 evolution activity, which shows a 19.2-fold increase in contrast to pristine g-C3N4, accompanying with a high apparent quantum efficiency of 11.9% at 420 +/- 15 nm. Experimental and OFT calculations results co-disclose that the aforementioned advantageous factors account for the profoundly boosted photooxidation and photoreduction capabilities of g-C3N4 under visible light. The present work may furnish a bottom-up tactic for integrally advancing g-C3N4, and also hold huge promise to be extended to other layered materials for photochemical or photoelectrochemical applications. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000390965000045

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Pinna, Nicola	G-2307-2010	
Zhang, Tierui	D-1633-2011	0000-0002-7948-9413
Dong, Fan	H-1449-2011	0000-0003-2890-9964
Reshak, Ali	B-8649-2008	0000-0001-9426-8363
Ye, Liqun		0000-0001-6410-689X
Pinna, Nicola		0000-0003-1273-803X

ISSN: 0926-3373

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Record 103 of 491

Title: Low- and high-energy spectroscopy of O-17 and F-17 within a microscopic multiphonon approach

Author(s): De Gregorio, G (De Gregorio, G.); Knapp, F (Knapp, F.); Lo Iudice, N (Lo Iudice, N.); Vesely, P (Vesely, P.)

Source: PHYSICAL REVIEW C **Volume:** 95 **Issue:** 3 **Article Number:** 034327 **DOI:** 10.1103/PhysRevC.95.034327 **Published:** MAR 30 2017

Abstract: The extension of an equation of motion phonon method to odd nuclei is described step by step. Equations of motion are first constructed and solved to generate an orthonormal basis of correlated n-phonon states (n = 0,1,2,...), built of constituent Tamm-Dancoff phonons, describing the excitations of a doubly magic core. Analogous equations are then derived within a subspace spanned by a valence particle coupled to the n-phonon core states and solved iteratively to yield a basis of correlated orthonormal multiphonon particle-core states. The basis so constructed is used to solve the full eigenvalue problem for the odd system. The formalism does not rely on approximations but lends itself naturally to simplifying assumptions, as illustrated by its application to O-17 and F-17. Self-consistent calculations using a chiral Hamiltonian in a space encompassing up to three-phonon basis states generate spectra having a high level density, comparable to that observed experimentally. The spectroscopic properties are investigated at low energy through the calculation of moments, electromagnetic and beta-decay transition strengths, and at intermediate and high energy through the computation of the electric-dipole spectra and pygmy and giant dipole resonance cross sections. The analysis of the particle-phonon composition of the eigenfunctions contributes to clarify the mechanism of excitation of levels and resonances and gives unique insights into their nature.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290
De Gregorio, Giovanni		0000-0003-0253-915X

ISSN: 2469-9985

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Record 104 of 491

Title: Ab initio explanation of disorder and off-stoichiometry in Fe-Mn-Al-C kappa carbides

Author(s): Dey, P (Dey, Poulumi); Nazarov, R (Nazarov, Roman); Dutta, B (Dutta, Biswanath); Yao, M (Yao, Mengji); Herbig, M (Herbig, Michael); Friak, M (Friak, Martin); Hickel, T (Hickel, Tilmann); Raabe, D (Raabe, Dierk); Neugebauer, J (Neugebauer, Joerg)

Source: PHYSICAL REVIEW B **Volume:** 95 **Issue:** 10 **Article Number:** 104108 **DOI:** 10.1103/PhysRevB.95.104108 **Published:** MAR 22 2017

Abstract: Carbides play a central role for the strength and ductility in many materials. Simulating the impact of these precipitates on the mechanical performance requires knowledge about their atomic configuration. In particular, the C content is often observed to substantially deviate from the ideal stoichiometric composition. In thiswork, we focus on Fe-Mn-Al-C steels, for which we determined the composition of the nanosized. carbides (Fe, Mn)(3)AlC by atom probe tomography in comparison to larger precipitates located in grain boundaries. Combining density functional theory with thermodynamic concepts, we first determine the critical temperatures for the presence of chemical and magnetic disorder in these carbides. Second, the experimentally observed reduction of the C content is explained as a compromise between the gain in chemical energy during partitioning and the elastic strains emerging in coherent microstructures.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Herbig, Michael	O-1063-2013	

Dutta, Biswanath	T-2162-2017	0000-0003-4675-1646
Hickel, Tilmann		0000-0003-0698-4891

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Record 105 of 491

Title: Reducing the number of mean-square deviation calculations with floating close structure in metadynamics
Author(s): Pazurikova, J (Pazurikova, Jana); Krenek, A (Krenek, Ales); Spiwok, V (Spiwok, Vojtech); Simkova, M (Simkova, Maria)
Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 146 **Issue:** 11 **Article Number:** 115101 **DOI:** 10.1063/1.4978296 **Published:** MAR 21 2017
Abstract: Metadynamics is an important collective-coordinate-based enhanced sampling simulation method. Its performance depends significantly on the capability of collective coordinates to describe the studied molecular processes. Collective coordinates based on comparison with reference landmark structures can be used to enhance sampling in highly complex systems; however, they may slow down simulations due to high number of structure-structure distance (e.g., mean-square deviation) calculations. Here we introduce an approximation of root-mean-square or mean-square deviation that significantly reduces numbers of computationally expensive operations. We evaluate its accuracy and theoretical performance gain with metadynamics simulations on two molecular systems. Published by AIP Publishing.
Accession Number: WOS:000397313600032
PubMed ID: 28330370
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Krenek, Ales	I-1311-2016	0000-0002-3395-3196
Spiwok, Vojtech	A-7747-2008	0000-0001-8108-2033

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Record 106 of 491

Title: Structure of deformed wing virus, a major honey bee pathogen
Author(s): Skubnik, K (Skubnik, Karel); Novacek, J (Novacek, Jiri); Fuzik, T (Fuezik, Tibor); Pridal, A (Pridal, Antonin); Paxton, RJ (Paxton, Robert J.); Plevka, P (Plevka, Pavel)
Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA **Volume:** 114 **Issue:** 12 **Pages:** 3210-3215 **DOI:** 10.1073/pnas.1615695114 **Published:** MAR 21 2017
Abstract: The worldwide population of western honey bees (Apis mellifera) is under pressure from habitat loss, environmental stress, and pathogens, particularly viruses that cause lethal epidemics. Deformed wing virus (DWV) from the family Iflaviridae, together with its vector, the mite Varroa destructor, is likely the major threat to the world's honey bees. However, lack of knowledge of the atomic structures of iflaviruses has hindered the development of effective treatments against them. Here, we present the virion structures of DWV determined to a resolution of 3.1 angstrom using cryo-electron microscopy and 3.8 angstrom by X-ray crystallography. The C-terminal extension of capsid protein VP3 folds into a globular protruding (P) domain, exposed on the virion surface. The P domain contains an Asp-His-Ser catalytic triad that is, together with five residues that are spatially close, conserved among iflaviruses. These residues may participate in receptor binding or provide the protease, lipase, or esterase activity required for entry of the virus into a host cell. Furthermore, nucleotides of the DWV RNA genome interact with VP3 subunits. The capsid protein residues involved in the RNA binding are conserved among honey bee iflaviruses, suggesting a putative role of the genome in stabilizing the virion or facilitating capsid assembly. Identifying the RNA-binding and putative catalytic sites within the DWV virion structure enables future analyses of how DWV and other iflaviruses infect insect cells and also opens up possibilities for the development of antiviral treatments.
Accession Number: WOS:000396893600075
PubMed ID: 28270616
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fuzik, Tibor	J-2684-2017	0000-0002-1190-0210
Pridal, Antonin	S-5171-2017	0000-0002-5798-6785
Plevka, Pavel	H-8661-2014	0000-0003-4215-3315

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Record 107 of 491

Title: Bias cancellation in one-determinant fixed-node diffusion Monte Carlo: Insights from fermionic occupation numbers
Author(s): Dubecky, M (Dubecky, Matus)
Source: PHYSICAL REVIEW E **Volume:** 95 **Issue:** 3 **Article Number:** 033308 **DOI:** 10.1103/PhysRevE.95.033308 **Published:** MAR 15 2017
Abstract: The accuracy of the fixed-node diffusion Monte Carlo (FNDMC) depends on the node location of the supplied trial state psi(T). The practical FNDMC approaches available for large systems rely on compact yet effective psi(T), most often containing an explicitly correlated single Slater determinant (SD). However, SD nodes may be better suited to one system than to another, which may possibly lead to inaccurate FNDMC energy differences. It remains a challenge how to estimate nonequivalence or appropriateness of SDs. Here we use the differences of a measure based on the Euclidean distance between the natural orbital occupation number (NOON) vector of the SD and the exact solution in the NOON vector space, which can be viewed as a measure of SD nonequivalence and as a qualitative measure of the expected degree of nondynamic-correlation-related bias in FNDMC energy differences. This is explored on a set of small noncovalent complexes and covalent bond breaking of Si-2 vs N-2. It turns out that NOON-based measures well reflect the magnitude and sign of the bias present in the data available, thus providing insights into the nature of bias cancellation in SD FNDMC energy differences.
Accession Number: WOS:000396283700007
PubMed ID: 28415179
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dubecky, Matus	P-1720-2016	

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Record 108 of 491

Title: Electric Control of Dirac Quasiparticles by Spin-Orbit Torque in an Antiferromagnet
Author(s): Smejkal, L (Smejkal, L.); Zelezny, J (Zelezny, J.); Sinova, J (Sinova, J.); Jungwirth, T (Jungwirth, T.)
Source: PHYSICAL REVIEW LETTERS **Volume:** 118 **Issue:** 10 **Article Number:** 106402 **DOI:** 10.1103/PhysRevLett.118.106402 **Published:** MAR 6 2017
Abstract: Spin orbitronics and Dirac quasiparticles are two fields of condensed matter physics initiated independently about a decade ago. Here we predict that Dirac quasiparticles can be controlled by the spin-orbit torque reorientation of the Neel vector in an antiferromagnet. Using CuMnAs as an example, we formulate symmetry criteria allowing for the coexistence of topological Dirac quasiparticles and Neel spin-orbit torques. We identify the nonsymmorphic crystal symmetry protection of Dirac band crossings whose on and off switching is mediated by the Neel vector reorientation. We predict that this concept verified by minimal model and density functional calculations in the CuMnAs semimetal antiferromagnet can lead to a topological metal-insulator transition driven by the Neel vector and to the topological anisotropic magnetoresistance.
Accession Number: WOS:000396046100007
PubMed ID: 28339249
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sinova, Jairo	G-9071-2014	0000-0002-9490-2333
Zelezny, Jakub	G-5276-2014	0000-0001-9471-0078

ISSN: 0031-9007
eISSN: 1079-7114

Record 109 of 491

Title: The cyanobacterial metabolite nocuolin A is a natural oxadiazine that triggers apoptosis in human cancer cells

Author(s): Voracova, K (Voracova, Katerina); Hajek, J (Hajek, Jan); Mares, J (Mares, Jan); Urajova, P (Urajova, Petra); Kuzma, M (Kuzma, Marek); Cheel, J (Cheel, Jose); Villunger, A (Villunger, Andreas); Kapuscik, A (Kapuscik, Alexandra); Bally, M (Bally, Marcel); Novak, P (Novak, Petr); Kabelac, M (Kabelac, Martin); Krumschnabel, G (Krumschnabel, Gerhard); Lukes, M (Lukes, Martin); Voloshko, L (Voloshko, Ludmila); Kopecky, J (Kopecky, Jiri); Hrouzek, P (Hrouzek, Pavel)

Source: PLOS ONE **Volume:** 12 **Issue:** 3 **Article Number:** e0172850 **DOI:** 10.1371/journal.pone.0172850 **Published:** MAR 2 2017

Abstract: Oxadiazines are heterocyclic compounds containing N-N-O or N-N-C-O system within a six membered ring. These structures have been up to now exclusively prepared via organic synthesis. Here, we report the discovery of a natural oxadiazine nocuolin A (NoA) that has a unique structure based on 1,2,3-oxadiazine. We have identified this compound in three independent cyanobacterial strains of genera Nostoc, Nodularia, and Anabaena and recognized the putative gene clusters for NoA biosynthesis in their genomes. Its structure was characterized using a combination of NMR, HRMS and FTIR methods. The compound was first isolated as a positive hit during screening for apoptotic inducers in crude cyanobacterial extracts. We demonstrated that NoA-induced cell death has attributes of caspase-dependent apoptosis. Moreover, NoA exhibits a potent anti-proliferative activity (0.7-4.5 mu M) against several human cancer lines, with p53-mutated cell lines being even more sensitive. Since cancers bearing p53 mutations are resistant to several conventional anti-cancer drugs, NoA may offer a new scaffold for the development of drugs that have the potential to target tumor cells independent of their p53 status. As no analogous type of compound was previously described in the nature, NoA establishes a novel class of bioactive secondary metabolites.

Accession Number: WOS:000396011300042

PubMed ID: 28253280

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kuzma, Marek	F-5468-2015	0000-0001-7415-2734
Urajova, Petra	I-1663-2014	
Cheel, Jose	J-8401-2014	0000-0001-5789-9297
Mares, Jan	B-2395-2009	0000-0002-5745-7023
Novak, Petr	F-9655-2014	0000-0001-8688-529X

ISSN: 1932-6203

Record 110 of 491

Title: Non-coding RNA may be associated with cytoplasmic male sterility in Silene vulgaris

Author(s): Stone, JD (Stone, James D.); Kolouskova, P (Kolouskova, Pavla); Sloan, DB (Sloan, Daniel B.); Storchova, H (Storchova, Helena)

Source: JOURNAL OF EXPERIMENTAL BOTANY **Volume:** 68 **Issue:** 7 **Pages:** 1599-1612 **DOI:** 10.1093/jxb/erx057 **Published:** MAR 2017

Abstract: Cytoplasmic male sterility (CMS) is a widespread phenomenon in flowering plants caused by mitochondrial (mt) genes. CMS genes typically encode novel proteins that interfere with mt functions and can be silenced by nuclear fertility-restorer genes. Although the molecular basis of CMS is well established in a number of crop systems, our understanding of it in natural populations is far more limited. To identify CMS genes in a gynodioecious plant, Silene vulgaris, we constructed mt transcriptomes and compared transcript levels and RNA editing patterns in floral bud tissue from female and hermaphrodite full siblings. The transcriptomes from female and hermaphrodite individuals were very similar overall with respect to variation in levels of transcript abundance across the genome, the extent of RNA editing, and the order in which RNA editing and intron splicing events occurred. We found only a single genomic region that was highly overexpressed and differentially edited in females relative to hermaphrodites. This region is not located near any other transcribed elements and lacks an open-reading frame (ORF) of even moderate size. To our knowledge, this transcript would represent the first non-coding mt RNA associated with CMS in plants and is, therefore, an important target for future functional validation studies.

Accession Number: WOS:000400341800019

PubMed ID: 28369520

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Stone, James		0000-0002-4636-5158

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Record 111 of 491

Title: Virion Structure of Black Queen Cell Virus, a Common Honeybee Pathogen

Author(s): Spurny, R (Spurny, Radovan); Pridal, A (Pridal, Antonin); Palkova, L (Palkova, Lenka); Kiem, HKT (Hoa Khanh Tran Kiem); de Miranda, JR (de Miranda, Joachim R.); Plevka, P (Plevka, Pavel)

Source: JOURNAL OF VIROLOGY **Volume:** 91 **Issue:** 6 **Article Number:** UNSP e02100-16 **DOI:** 10.1128/JVI.02100-16 **Published:** MAR 2017

Abstract: Viral diseases are a major threat to honeybee (Apis mellifera) populations worldwide and therefore an important factor in reliable crop pollination and food security. Black queen cell virus (BQCV) is the etiological agent of a fatal disease of honeybee queen larvae and pupae. The virus belongs to the genus Triatovirus from the family Dicistroviridae, which is part of the order Picornavirales. Here we present a crystal structure of BQCV determined to a resolution of 3.4 angstrom. The virion is formed by 60 copies of each of the major capsid proteins VP1, VP2, and VP3; however, there is no density corresponding to a 75-residue-long minor capsid protein VP4 encoded by the BQCV genome. We show that the VP4 subunits are present in the crystallized virions that are infectious. This aspect of the BQCV virion is similar to that of the previously characterized triatoma virus and supports the recent establishment of the separate genus Triatovirus within the family Dicistroviridae. The C terminus of VP1 and CD loops of capsid proteins VP1 and VP3 of BQCV form 34-angstrom-tall finger-like protrusions at the virion surface. The protrusions are larger than those of related dicistroviruses.
IMPORTANCE The western honeybee is the most important pollinator of all, and it is required to sustain the agricultural production and biodiversity of wild flowering plants. However, honeybee populations worldwide are suffering from virus infections that cause colony losses. One of the most common, and least known, honeybee pathogens is black queen cell virus (BQCV), which at high titers causes queen larvae and pupae to turn black and die. Here we present the three-dimensional virion structure of BQCV, determined by X-ray crystallography. The structure of BQCV reveals large protrusions on the virion surface. Capsid protein VP1 of BQCV does not contain a hydrophobic pocket. Therefore, the BQCV virion structure provides evidence that capsid-binding antiviral compounds that can prevent the replication of vertebrate picornaviruses may be ineffective against honeybee virus infections.

Accession Number: WOS:000398098300016

PubMed ID: 28077635

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Pridal, Antonin	S-5171-2017	0000-0002-5798-6785
Plevka, Pavel	H-8661-2014	0000-0003-4215-3315

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Record 112 of 491

Title: Speeding up the multimedia feature extraction: a comparative study on the big data approach

Author(s): Mera, D (Mera, David); Batko, M (Batko, Michal); Zezula, P (Zezula, Pavel)

Source: MULTIMEDIA TOOLS AND APPLICATIONS **Volume:** 76 **Issue:** 5 **Pages:** 7497-7517 **DOI:** 10.1007/s11042-016-3415-1 **Published:** MAR 2017

Abstract: The current explosion of multimedia data is significantly increasing the amount of potential knowledge. However, to get to the actual information requires to apply novel content-based techniques which in turn require time consuming extraction of indexable features from the raw data. In order to deal with large datasets, this task needs to be parallelized. However, there are multiple approaches to choose from, each with its own benefits and drawbacks. There are also several parameters that must be taken into consideration, for example the amount of available resources, the size of the data and their availability. In this paper, we empirically evaluate and compare approaches based on Apache Hadoop, Apache Storm, Apache Spark, and Grid computing, employed to distribute the extraction task over an outsourced and distributed infrastructure.

Accession Number: WOS:000397278400062

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mera, David		0000-0002-0639-6574

ISSN: 1380-7501
eISSN: 1573-7721

Record 113 of 491
Title: Anion-pi Interactions in Flavoproteins Involve a Substantial Charge-Transfer Component
Author(s): Yurenko, YP (Yurenko, Yevgen P.); Bazzi, S (Bazzi, Sophia); Marek, R (Marek, Radek); Kozelka, J (Kozelka, Jiri)
Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 23 **Issue:** 14 **Pages:** 3246-3250 **DOI:** 10.1002/chem.201605307 **Published:** MAR 2017
Abstract: Anion-pi interactions have been shown to stabilize flavoproteins and to regulate the redox potential of the flavin cofactor. They are commonly attributed to electrostatic forces. Herein we show that anion-flavin interactions can have a substantial charge-transfer component. Our conclusion emanates from a multi-approach theoretical analysis and is backed by previously reported observations of absorption bands, originating from charge transfer between oxidized flavin and proximate cysteine thiolate groups. This partial covalency of anion-flavin contacts renders classical simulations of flavoproteins questionable.
Accession Number: WOS:000395775700002
PubMed ID: 28098402
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Yurenko, Yevgen	I-8022-2012	0000-0003-3925-0384
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Bazzi, Sophia		0000-0001-5885-3231

ISSN: 0947-6539
eISSN: 1521-3765

Record 114 of 491
Title: Practical Multicriteria Urban Bicycle Routing
Author(s): Hrncir, J (Hrncir, Jan); Zilecky, P (Zilecky, Pavol); Song, Q (Song, Qing); Jakob, M (Jakob, Michal)
Source: IEEE TRANSACTIONS ON INTELLIGENT TRANSPORTATION SYSTEMS **Volume:** 18 **Issue:** 3 **Pages:** 493-504 **DOI:** 10.1109/TITS.2016.2577047 **Published:** MAR 2017
Abstract: Increasing the adoption of cycling is crucial for achieving more sustainable urban mobility. Navigating larger cities on a bike is, however, often challenging due to the cities' fragmented cycling infrastructure and/or complex terrain topology. Cyclists would thus benefit from intelligent route planning that would help them discover routes that best suit their transport needs and preferences. Because of the many factors cyclists consider in deciding their routes, employing a multicriteria route search is vital for properly accounting for cyclists' route-choice criteria. A direct application of optimal multicriteria route search algorithms is, however, not feasible due to their prohibitive computational complexity. In this paper, we formalize a multicriteria bicycle routing problem and propose several heuristics for speeding up the multicriteria route search. We evaluate our method on a real-world cycleway network and show that speedups of up to four orders of magnitude over the standard multicriteria label-setting algorithm are possible with a reasonable loss of solution quality. Our results make it possible to practically deploy bicycle route planners capable of producing diverse high-quality route suggestions respecting multiple real-world route-choice criteria.
Accession Number: WOS:000396143200003
ISSN: 1524-9050
eISSN: 1558-0016

Record 115 of 491
Title: Insight into thiabendazole interaction with montmorillonite and organically modified montmorillonites
Author(s): Gamba, M (Gamba, Martina); Kovar, P (Kovar, Petr); Pospisil, M (Pospisil, Miroslav); Sanchez, RMT (Torres Sanchez, Rosa M.)
Source: APPLIED CLAY SCIENCE **Volume:** 137 **Pages:** 59-68 **DOI:** 10.1016/j.clay.2016.12.001 **Published:** MAR 1 2017
Abstract: The interactions of the fungicide, thiabendazole (TBZ) on montmorillonite (Mt) and organoclays synthesized from phosphatidylcholine (DSPC) and octadecyltrimethylammonium bromide (ODTMA) was investigated for water remediation. The affinity of TBZ on the surface of Mt and organoclays was evaluated by powder X-ray diffraction, X-ray photoelectron spectroscopy and the experimental results were also reinforced by molecular modelling in order to explore the surfaces arrangements. TBZ was protonated upon interaction with negative charged Mt and therefore this strong electrostatic interactions prevented it's desorption in water. Repulsive electrostatic interactions between the cationic surfactant ODTMA and the cationic form of TBZ on the outer surface of the ODTMA modified Mt resulted in high desorption values. In the DSPC modified Mt, TBZ was anchored within the surfactant chains and a small amount of interlayer water was released from the interlayer space. (C) 2016 Elsevier B.V. All rights reserved.
Accession Number: WOS:000393002300009
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Pospisil, Miroslav	A-2069-2012	0000-0002-5437-0141
Kovar, Petr	N-2780-2017	0000-0003-4246-0307
Torres Sanchez, Rosa Maria		0000-0002-9357-1210

ISSN: 0169-1317
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Record 116 of 491
Title: Conjugated Metallo-Supramolecular Polymers Containing a Phosphole Unit
Author(s): Vitvarova, T (Vitvarova, Tereza); Svoboda, J (Svoboda, Jan); Hissler, M (Hissler, Muriel); Vohlidal, J (Vohlidal, Jiri)
Source: ORGANOMETALLICS **Volume:** 36 **Issue:** 4 **Pages:** 777-786 **DOI:** 10.1021/acs.organomet.6b00822 **Published:** FEB 27 2017
Abstract: A new building block, TPT, composed of the substituted phosphole ring surrounded by two thiophene rings with 2,2':6',2"-terpyridine-4'-yl (tpy) end-groups, is prepared and assembled with metal ions (Co2+, Cu2+, Fe2+, Ni2+, and Zn2+) into metallo-supramolecular polymers (MSPs), and properties of both TPT and the MSPs are compared with those of their counterparts with terthiophene central blocks. A distinct red-shifting of the UV/vis band about by 60-100 nm proves the decrease in the bandgap energy due to replacing the thiophene-2,5-diyl with a phosphole-2,5-diyl central unit, which is due to the lowered aromaticity of phosphole ring compared to the aromaticity of thiophene ring. Assembling TPT with metal ions gives oligomeric chains comprising up to 10 unimeric units in dilute solutions. MSPs with Fe2+ and Ni2+ ion couplers exhibit very slow constitutional dynamics, while those with Cu2+ and Zn2+ ion couplers quite fast constitutional dynamics. A metal ligand charge transfer is observed only for Fe-2+-MSPs, while luminescence is observed only for. Zn2+-MSPs, mainly at an excess of Zn2+ ions, which indicates a positive effect of the end-capping of MSP chains with these ions.
Accession Number: WOS:000395226200003
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Svoboda, Jan	E-4750-2014	0000-0002-4989-4274
Vohlidal, Jiri		0000-0002-9412-2548

ISSN: 0276-7333
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Record 117 of 491
Title: Bambusuril as a One-Electron Donor for Photoinduced Electron Transfer to Methyl Viologen in Mixed Crystals
Author(s): Fiala, T (Fiala, Tomas); Ludvikova, L (Ludvikova, Lucie); Heger, D (Heger, Dominik); Svec, J (Svec, Jan); Slanina, T (Slanina, Tomas); Vetrakova, L (Vetrakova, L'ubica); Babiak, M (Babiak, Michal); Necas, M (Necas, Marek); Kulhanek, P (Kulhanek, Petr); Klan, P (Klan, Petr); Sindelar, V (Sindelar, Vladimir)
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 139 **Issue:** 7 **Pages:** 2597-2603 **DOI:** 10.1021/jacs.6b08589 **Published:** FEB 22 2017

Abstract: Methyl viologen hexafluorophosphate (MV2+center dot 2PF(6)(-)) and dodecamethylbambus[6]uril (BU6) form crystals in which the layers of viologen dications alternate with those of a 1:2 supramolecular complex of BU6 and PF6-. This arrangement allows for a one-electron reduction of MV2+ ions upon UV irradiation to form MV+center dot radical cations within the crystal structure with half-lives of several hours in air. The mechanism of this photoinduced electron transfer in the solid state and the origin of the long-lived charge-separated state were studied by steady-state and transient spectroscopies, cyclic voltammetry, and electron paramagnetic resonance spectroscopy. Our experiments are supported by quantum-chemical calculations showing that BU6 acts as a reductant. In addition, analogous photochemical behavior is also demonstrated on other MV2+/BU6 crystals containing either BF4- or Br- counterions.

Accession Number: WOS:000394829200016

PubMed ID: 28222609

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sindelar, Vladimir	H-9893-2012	0000-0003-0090-5961
Klan, Petr	H-1189-2012	0000-0001-6287-2742
Kulhanek, Petr	D-6884-2012	0000-0002-4152-6514
Fiala, Tomas	M-9409-2017	0000-0001-6949-4561
Necas, Marek	F-6833-2010	
Heger, Dominik	H-9934-2012	0000-0002-6881-8699
Vetrakova, Lubica	F-5040-2017	0000-0003-3536-1706

ISSN: 0002-7863

Record 118 of 491

Title: Chasing the Evasive Fe = O Stretch and the Spin State of the Iron(IV)-Oxo Complexes by Photodissociation Spectroscopy

Author(s): Andris, E (Andris, Erik); Navratil, R (Navratil, Rafael); Jasik, J (Jasik, Juraj); Terencio, T (Terencio, Thibault); Srnec, M (Srnec, Martin); Costas, M (Costas, Miguel); Roithova, J (Roithova, Jana)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 139 **Issue:** 7 **Pages:** 2757-2765 **DOI:** 10.1021/jacs.6b12291 **Published:** FEB 22 2017

Abstract: We demonstrate the application of infrared photodissocation spectroscopy for determination of the Fe = O stretching frequencies of high-valent iron(IV)-oxo complexes [(L)Fe(O)(X)](2+/+) (L = TMC, N4Py, PyTACN, and X = CH3CN, CF3SO3, ClO4, CF3COO, NO3, N-3). We show that the values determined by resonance Raman spectroscopy in acetonitrile solutions are on average 9 cm(-1) red-shifted with respect to unbiased gas-phase values. Furthermore, we show the assignment of the spin state of the complexes based on the vibrational modes of a coordinated anion and compare reactivities of various iron(IV)-oxo complexes generated as dications or monocations (bearing an anionic ligand). The coordinated anions can drastically affect the reactivity of the complex and should be taken into account when comparing reactivities of complexes bearing different ligands. Comparison of reactivities of [(PyTACN)Fe(O)(X)](+) generated in different spin states and bearing different anionic ligands X revealed that the nature of anion influences the reactivity more than the spin state. The triflate and perchlorate ligands tend to stabilize the quintet state of [(PyTACN)Fe(O)(X)](+), whereas trifluoroacetate and nitrate stabilize the triplet state of the complex.

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PubMed ID: 28125220

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Navratil, Rafael	O-4427-2017	0000-0003-3949-0185
Andris, Erik	O-2513-2017	0000-0002-9336-0157
Jasik, Juraj	O-1057-2017	0000-0002-1177-2837
Roithova, Jana		0000-0001-5144-0688
costas, Miquel		0000-0001-6326-8299

ISSN: 0002-7863

Record 119 of 491

Title: Reclassification of non-type strain Clostridium pasteurianum NRRL B-598 as Clostridium beijerinckii NRRL B-598

Author(s): Sedlar, K (Sedlar, Karel); Kolek, J (Kolek, Jan); Provaznik, I (Provaznik, Ivo); Patakova, P (Patakova, Petra)

Source: JOURNAL OF BIOTECHNOLOGY **Volume:** 244 **Pages:** 1-3 **DOI:** 10.1016/j.jbiotec.2017.01.003 **Published:** FEB 20 2017

Abstract: The complete genome sequence of non-type strain Clostridium pasteurianum NRRL B-598 was introduced last year; it is an oxygen tolerant, spore-forming, mesophilic heterofermentative bacterium with high hydrogen production and acetone-butanol fermentation ability. The basic genome statistics have shown its similarity to C. beijerinckii rather than the C. pasteurianum species. Here, we present a comparative analysis of the strain with several other complete clostridial genome sequences. Besides a 16S rRNA gene sequence comparison, digital DNA-DNA hybridization (dDDH) and phylogenomic analysis confirmed an inaccuracy of the taxonomic status of strain Clostridium pasteurianum NRRL B-598. Therefore, we suggest its reclassification to be Clostridium beijerinckii NRRL B-598. This is a specific strain and is not identical to other C. beijerinckii strains. This misclassification explains its unexpected behavior, different from other C. pasteurianum strains; it also permits better understanding of the bacterium for a future genetic manipulation that might increase its biofuel production potential. (C)2017 Elsevier B.V. All rights reserved.

Accession Number: WOS:000395222100001

PubMed ID: 28111164

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sedlar, Karel	K-1120-2014	0000-0002-8269-4020
Patakova, Petra	B-6404-2018	0000-0002-9410-4454
Provaznik, Ivo	F-4121-2012	0000-0002-3422-7938

ISSN: 0168-1656

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Record 120 of 491

Title: Interaction of the cesium cation with meso-octamethylcalix[4]pyrrole: Experimental and theoretical study

Author(s): Polasek, M (Polasek, Miroslav); Makrlik, E (Makrlik, Emanuel); Kvicala, J (Kvicala, Jaroslav); Krizova, V (Krizova, Vera); Vanura, P (Vanura, Petr)

Source: CHEMICAL PHYSICS LETTERS **Volume:** 670 **Pages:** 22-26 **DOI:** 10.1016/j.cplett.2016.12.044 **Published:** FEB 16 2017

Abstract: By using electrospray ionization mass spectrometry (ESI-MS), it was proven experimentally that the univalent cesium cation (cs(+)) forms with meso-octamethylcalix[4]pyrrole (abbrev. 1) the cationic complex species 1.Cs+. Further, applying quantum chemical DFT calculations, four different conformations of the resulting complex 1.Cs+ were derived. It means that under the present experimental conditions, this ligand I can be considered as a macrocyclic receptor for the cesium cation. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000393721900005

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Polasek, Miroslav	G-7217-2014	
Krizova, Vera	O-6658-2017	0000-0002-8107-5500

ISSN: 0009-2614

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Record 121 of 491

Title: Considerations and complications of mapping small RNA high-throughput data to transposable elements

Author(s): Bousios, A (Bousios, Alexandros); Gaut, BS (Gaut, Brandon S.); Darzentas, N (Darzentas, Nikos)

Source: MOBILE DNA **Volume:** 8 **Article Number:** 3 **DOI:** 10.1186/s13100-017-0086-z **Published:** FEB 15 2017

Abstract: Background: High-throughput sequencing (HTS) has revolutionized the way in which epigenetic research is conducted. When coupled with fully-sequenced genomes, millions of small RNA (sRNA) reads are mapped to regions of interest and the results scrutinized for clues about epigenetic mechanisms. However, this approach requires careful consideration in regards to experimental design, especially when one investigates repetitive parts of genomes such as transposable elements (TEs), or when such genomes are large, as is often the case in plants.
Results: Here, in an attempt to shed light on complications of mapping sRNAs to TEs, we focus on the 2,300 Mb maize genome, 85% of which is derived from TEs, and scrutinize methodological strategies that are commonly employed in TE studies. These include choices for the reference dataset, the normalization of multiply mapping sRNAs, and the selection among sRNA metrics. We further examine how these choices influence the relationship between sRNAs and the critical feature of TE age, and contrast their effect on low copy genomic regions and other popular HTS data.
Conclusions: Based on our analyses, we share a series of take-home messages that may help with the design, implementation, and interpretation of high-throughput TE epigenetic studies specifically, but our conclusions may also apply to any work that involves analysis of HTS data.

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PubMed ID: 28228849

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bousios, Alexandros		0000-0002-8005-6949

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Record 122 of 491

Title: Interaction of irradiation-induced prismatic dislocation loops with free surfaces in tungsten

Author(s): Fikar, J (Fikar, Jan); Groger, R (Groeger, Roman); Schaublin, R (Schaeublin, Robin)

Source: NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS **Volume:** 393 **Pages:** 186-189 **DOI:** 10.1016/j.nimb.2016.10.006 **Published:** FEB 15 2017

Abstract: The prismatit dislocation loops appear in metals as a result of high-energy irradiation. Understanding their formation and interaction is important for quantification of irradiation-induced deterioration of mechanical properties. Characterization of dislocation loops in thin foils is commonly made using transmission electron microscopy (TEM), but the results are inevitably influenced by the proximity of free surfaces. The prismatic loops are attracted to free surfaces by image forces. Depending on the type, size and depth of the loop in the foil, they can escape to the free surface, thus invalidating TEM observations and conclusions. In this article small prismatic hexagonal and circular dislocation loops in tungsten with the Burgers vectors 1/2(111) and (100) are studied by molecular statics simulations using three embedded atom method (EAM) potentials. The calculated image forces are compared to known elastic solutions. A particular attention is paid to the critical stress to move edge dislocations. The escape of the loop to the free surface is quantified by a combination of atomistic simulations and elastic calculations. For example, for the 1/2(1 1 1) loop with diameter 7.4 nm in a 55 nm thick foil we calculated that about one half of the loops will escape to the free surface. This implies that TEM observations detect only approx. 50% of the loops that were originally present in the foil. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000394194500041

Conference Title: 13th International Conference on Computer Simulation of Radiation Effects in Solids (COSIRES)

Conference Date: JUN 19-24, 2016

Conference Location: Loughborough Univ, Loughborough, ENGLAND

Conference Sponsors: Inst Phys, CCP5, IAEA, UK Engn & Phys Sci Res Council

Conference Host: Loughborough Univ

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Record 123 of 491

Title: Comparative first-principles calculations of the electronic, optical, elastic and thermodynamic properties of XCaF3 (X = K, Rb, Cs) cubic perovskites

Author(s): Li, L (Li, Li); Wang, YJ (Wang, Y. J.); Liu, DX (Liu, D. -X.); Ma, CG (Ma, C. -G.); Brik, MG (Brik, M. G.); Suchocki, A (Suchocki, A.); Piasecki, M (Piasecki, M.); Reshak, AH (Reshak, A. H.)

Source: MATERIALS CHEMISTRY AND PHYSICS **Volume:** 188 **Pages:** 39-48 **DOI:** 10.1016/j.matchemphys.2016.12.033 **Published:** FEB 15 2017

Abstract: Three fluoroperovskites with the general formula XCaF3 (X = K, Rb, Cs) have been systematically studied using the first-principles methods. The structural, electronic, optical, elastic and thermodynamic properties of these three compounds were calculated at the ambient and elevated hydrostatic pressure. Variation of all these properties with pressure was analyzed; it was shown that the structural and elastic constants change linearly with increased pressure, whereas the calculated band gaps follow the quadratic dependence on pressure. Influence of the first cation variation (K - Rb - Cs) on these properties was discussed. Elastic anisotropy (directional dependence of the Young moduli) of these compounds was modeled and analyzed for the first time. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000393253000006

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ma, Chong-Geng	G-3311-2010	0000-0001-8090-1738
Reshak, Ali	B-8649-2008	0000-0001-9426-8363
Wang, Yongjie	V-6640-2017	0000-0002-5580-8555
Piasecki, Michal	J-8302-2015	0000-0003-1040-8811
Suchocki, Andrzej	A-4244-2016	
Brik, Mikhail	C-4971-2009	0000-0003-2841-2763

ISSN: 0254-0584

eISSN: 1879-3312

Record 124 of 491

Title: Cation-pi interaction of the univalent silver cation with meso-octamethylcalix[4]pyrrole: Experimental and theoretical study

Author(s): Polasek, M (Polasek, Miroslav); Kvicala, J (Kvicala, Jaroslav); Makrlik, E (Makrlik, Emanuel); Krizova, V (Krizova, Vera); Vanura, P (Vanura, Petr)

Source: JOURNAL OF MOLECULAR STRUCTURE **Volume:** 1130 **Pages:** 408-413 **DOI:** 10.1016/j.molstruc.2016.10.003 **Published:** FEB 15 2017

Abstract: By using electrospray ionization mass spectrometry (ESI-MS), it was proven experimentally that the univalent silver cation Ag+ forms with meso-octamethylcalix[4]pyrrole (abbrev. 1) the cationic complex species 1 center dot Ag+. Further, applying quantum chemical DFT calculations, four different conformations of the resulting complex 1 center dot Ag+ were derived. It means that under the present experimental conditions, this ligand 1 can be considered as a macrocyclic receptor for the silver cation. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000390731800049

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Krizova, Vera	O-6658-2017	0000-0002-8107-5500
Polasek, Miroslav	G-7217-2014	

ISSN: 0022-2860

eISSN: 1872-8014

Record 125 of 491

Title: Ground-state correlations within a nonperturbative approach

Author(s): De Gregorio, G (De Gregorio, G.); Herko, J (Herko, J.); Knapp, F (Knapp, F.); Lo Iudice, N (Lo Iudice, N.); Vesely, P (Vesely, P.)

Source: PHYSICAL REVIEW C **Volume:** 95 **Issue:** 2 **Article Number:** 024306 **DOI:** 10.1103/PhysRevC.95.024306 **Published:** FEB 7 2017

Abstract: The contribution of the two-phonon configurations to the ground state of He-4 and O-16 is evaluated nonperturbatively using a Hartree-Fock basis within an equation-of-motion phonon method using a nucleon-nucleon optimized chiral potential. Convergence properties of energies and root-mean-square radii versus the harmonic oscillator frequency and space dimensions are investigated. The comparison with the second-order perturbation theory calculations shows that the higher-order terms have an appreciable repulsive effect and yield too-small binding energies and nuclear radii. It is argued that four-phonon configurations, through their strong coupling to two phonons, may provide most of the attractive contribution necessary for filling the gap between theoretical and experimental quantities. Possible strategies for accomplishing such a challenging task are discussed.

Accession Number: WOS:000393501800003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290
De Gregorio, Giovanni		0000-0003-0253-915X

ISSN: 2469-9985
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Record 126 of 491

Title: Proteomics offers insight to the mechanism behind Pisum sativum L. response to pea seed-borne mosaic virus (PSbMV)

Author(s): Cerna, H (Cerna, Hana); Cerny, M (Cerny, Martin); Habanova, H (Habanova, Hana); Safarova, D (Safarova, Dana); Abushamsiya, K (Abushamsiya, Kifah); Navratil, M (Navratil, Milan); Brzobohaty, B (Brzobohaty, Bretislav)

Source: JOURNAL OF PROTEOMICS **Volume:** 153 **Special Issue:** SI **Pages:** 78-88 **DOI:** 10.1016/j.jprot.2016.05.018 **Published:** FEB 5 2017

Abstract: Pea seed-borne mosaic virus (PSbMV) significantly reduces yields in a broad spectra of legumes. The eukaryotic translation initiation factor has been shown to confer resistance to this pathogen, thus implying that translation and proteome dynamics play a role in resistance. This study presents the results of a proteome-wide analysis of Pisum sativum L response to PSbMV infection. LC-MS profiling of two contrasting pea cultivars, resistant (B99) and susceptible (Raman) to PSbMV infection, detected >2300 proteins, 116 of which responded to PSbMV ten and/or twenty days post-inoculation. These differentially abundant proteins are involved in number of processes that have previously been reported in the plant-pathogen response, including protein and amino acid metabolism, stress signaling, redox homeostasis, carbohydrate metabolism, and lipid metabolism. We complemented our proteome-wide analysis work with targeted analyses of free amino acids and selected small molecules, fatty acid profiling, and enzyme activity assays. Data from these additional experiments support our findings and validate the biological relevance of the observed proteome changes. We found surprising similarities in the resistant and susceptible cultivars, which implies that a seemingly unaffected plant, with no detectable levels of PSbMV, actively suppresses viral replication.
Biological significance: Plant resistance to PSbMV is connected to translation initiation factors, yet the processes involved are still poorly understood at the proteome level. To the best of our knowledge, this is the first survey of the global proteomic response to PSbMV in plants. The combination of label-free LC-MS profiling and two contrasting cultivars (resistant and susceptible) provided highly sensitive snapshots of protein abundance in response to PSbMV infection. PSbMV is a member of the largest family of plant viruses and our results are in accordance with previously characterized potyvirus-responsive proteomes. Hence, the results of this study can further extend our knowledge about these pathogens. We also show that even though no viral replication is detected in the PSbMV-resistant cultivar B99, it is still significantly affected by PSbMV inoculation. (C) 2016 Elsevier B.V. All rights reserved.

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PubMed ID: 27235724
Conference Title: 10th Central and Eastern European Proteomics Conference (CEEPC)
Conference Date: OCT 11-14, 2016
Conference Location: Hungarian Acad Sci, Res Ctr Nat Sci, Budapest, HUNGARY
Conference Host: Hungarian Acad Sci, Res Ctr Nat Sci

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cerny, Martin	D-7226-2012	
Cerny, Martin		0000-0002-0651-4219

ISSN: 1874-3919
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Record 127 of 491

Title: Temperature dependent growth rates of the upper-hybrid waves and solar radio zebra patterns

Author(s): Benacek, J (Benacek, J.); Karlicky, M (Karlicky, M.); Yasnov, LV (Yasnov, L. V.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 598 **Article Number:** A106 **DOI:** 10.1051/0004-6361/201629717 **Published:** FEB 2017

Abstract: Context. The zebra patterns observed in solar radio emission are very important for flare plasma diagnostics. The most promising model of these patterns is based on double plasma resonance instability, which generates upper-hybrid waves, which can be then transformed into the zebra emission.
Aims. We aim to study in detail the double plasma resonance instability of hot electrons, together with a much denser thermal background plasma. In particular, we analyse how the growth rate of the instability depends on the temperature of both the hot plasma and background plasma components.
Methods. We numerically integrated the analysed model equations, using Python and Wolfram Mathematica.
Results. We found that the growth-rate maxima of the upper-hybrid waves for non-zero temperatures of both the hot and background plasma are shifted towards lower frequencies comparing to the zero temperature case. This shift increases with an increase of the harmonic number s of the electron cyclotron frequency and temperatures of both hot and background plasma components. We show how this shift changes values of the magnetic field strength estimated from observed zebras. We confirmed that for a relatively low hot electron temperature, the dependence of growth rate vs. both the ratio of the electron plasma and electron cyclotron frequencies expresse distinct peaks, and by increasing this temperature these peaks become smoothed. We found that in some cases, the values of wave number vector components for the upper-hybrid wave for the maximal growth rate strongly deviate from their analytical estimations. We confirmed the validity of the assumptions used when deriving model equations.

Accession Number: WOS:000394465000105

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Karlicky, Marian	G-9023-2014	
Yasnov, Leonid	L-8265-2013	0000-0001-7164-9382

ISSN: 1432-0746

Record 128 of 491

Title: New adenoviruses from new primate hosts - growing diversity reveals taxonomic weak points

Author(s): Dadakova, E (Dadakova, Eva); Chrudimsky, T (Chrudimsky, Tomas); Brozova, K (Brozova, Kristyna); Modry, D (Modry, David); Celer, V (Celer, Vladimir); Hrazdilova, K (Hrazdilova, Kristyna)

Source: MOLECULAR PHYLOGENETICS AND EVOLUTION **Volume:** 107 **Pages:** 305-307 **DOI:** 10.1016/j.ympev.2016.11.013 **Published:** FEB 2017

Abstract: The knowledge of the closest human relatives of human adenoviruses (AdVs) such as adenoviruses found in nonhuman primates is still limited, despite the growing importance of adenoviruses in vaccine development, gene and cancer therapy. We examined 153 stool samples of 17 non-human primate species and detected adenoviral DNA sequences of DNA polymerase (DPOL) gene in 54 samples (35%), originating from 12 out of 17 primate species. We further sequenced 15 hexon gene fragments and based on the phylogenetic analysis we propose two new provisional species SAdV-H and SAdV-I. Our study shows extensive diversity of adenoviral strains forming separate clades often from closely related host species from old world monkeys suggesting the existence of new species of AdVs and shows the necessity for clear ICTV guidelines for final establishment of so far provisional AdV species. (C) 2016 Elsevier Inc. All rights reserved.

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PubMed ID: 27894993
ISSN: 1055-7903
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Record 129 of 491

Title: ARResT/Interrogate: an interactive immunoprofiler for IG/TR NGS data

Author(s): Bystry, V (Bystry, Vojtech); Reigl, T (Reigl, Tomas); Krejci, A (Krejci, Adam); Demko, M (Demko, Martin); Hanakova, B (Hanakova, Barbora); Grioni, A (Grioni, Andrea); Knecht, H (Knecht, Henrik); Schlitt, M (Schlitt, Max); Dreger, P (Dreger, Peter); Sellner, L (Sellner, Leopold); Herrmann, D (Herrmann, Dietrich); Pingeon, M (Pingeon, Marine); Boudjoghra, M (Boudjoghra, Myriam); Rijntjes, J (Rijntjes, Jos); Pott, C (Pott, Christiane); Langerak, AW (Langerak, Anton W.); Groenen, PJTA (Groenen, Patricia J. T. A.); Davi, F (Davi, Frederic); Bruggemann, M (Brueggemann, Monika); Darzentas, N (Darzentas, Nikos)

Group Author(s): EuroClonality- NGS

Source: BIOINFORMATICS **Volume:** 33 **Issue:** 3 **Pages:** 435-437 **DOI:** 10.1093/bioinformatics/btw634 **Published:** FEB 1 2017

Abstract: Motivation: The study of immunoglobulins and T cell receptors using next-generation sequencing has finally allowed exploring immune repertoires and responses in their immense variability and complexity. Unsurprisingly, their analysis and interpretation is a highly convoluted task.
Results: We thus implemented ARResT/Interrogate, a web-based, interactive application. It can organize and filter large amounts of immunogenetic data by numerous criteria, calculate several relevant statistics, and present results in the form of multiple interconnected visualizations.

Accession Number: WOS:000397260800018

PubMed ID: 28172348

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Groenen, p	L-4336-2015	0000-0003-4314-228X
Sellner, Leopold		0000-0002-7893-401X

ISSN: 1367-4803

eISSN: 1460-2059

Record 130 of 491

Title: Joint accurate time and stable frequency distribution infrastructure sharing fiber footprint with research network

Author(s): Vojtech, J (Vojtech, Josef); Slapak, M (Slapak, Martin); Skoda, P (Skoda, Pavel); Radil, J (Radil, Jan); Havlis, O (Havlis, Ondrej); Altmann, M (Altmann, Michal); Munster, P (Munster, Petr); Velc, R (Velc, Radek); Kundrat, J (Kundrat, Jan); Altmannova, L (Altmannova, Lada); Vohnout, R (Vohnout, Rudolf); Horvath, T (Horvath, Tomas); Hula, M (Hula, Miloslav); Smotlacha, V (Smotlacha, Vladimir); Cizek, M (Cizek, Martin); Pravdova, L (Pravdova, Lenka); Rerucha, S (Rerucha, Simon); Hrabina, J (Hrabina, Jan); Cip, O (Cip, Ondrej)

Source: OPTICAL ENGINEERING **Volume:** 56 **Issue:** 2 **Article Number:** 027101 **DOI:** 10.1117/1.OE.56.2.027101 **Published:** FEB 2017

Abstract: The infrastructure essentialities for accurate time and stable frequency distribution are presented. Our solution is based on sharing fibers for a research and educational network carrying live data traffic with time and frequency transfer in parallel. Accurate time and stable frequency transmission uses mainly dark channels amplified by dedicated bidirectional amplifiers with the same propagation path for both directions of transmission. This paper targets challenges related to bidirectional transmission, particularly, directional nonreciprocities. (C) The Authors.

Accession Number: WOS:000397206800040

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cip, Ondrej	D-8547-2012	
Cizek, Martin	I-7839-2012	0000-0001-6938-3423
Rerucha, Simon	D-6924-2012	0000-0002-2026-5159
Hrabina, Jan	A-7297-2012	0000-0001-6030-7854
Pravdova, Lenka	D-7682-2015	

ISSN: 0091-3286

eISSN: 1560-2303

Record 131 of 491

Title: Cryo-electron Microscopy Study of the Genome Release of the Dicistrovirus Israeli Acute Bee Paralysis Virus

Author(s): Mullapudi, E (Mullapudi, Edukondalu); Fuzik, T (Fuezik, Tibor); Pridal, A (Pridal, Antonin); Plevka, P (Plevka, Pavel)

Source: JOURNAL OF VIROLOGY **Volume:** 91 **Issue:** 4 **Article Number:** UNSP e02060 **DOI:** 10.1128/JVI.02060-16 **Published:** FEB 2017

Abstract: Viruses of the family Dicistroviridae can cause substantial economic damage by infecting agriculturally important insects. Israeli acute bee paralysis virus (IAPV) causes honeybee colony collapse disorder in the United States. High-resolution molecular details of the genome delivery mechanism of dicistroviruses are unknown. Here we present a cryo-electron microscopy analysis of IAPV virions induced to release their genomes in vitro. We determined structures of full IAPV virions primed to release their genomes to a resolution of 3.3 angstrom and of empty capsids to a resolution of 3.9 angstrom. We show that IAPV does not form expanded A particles before genome release as in the case of related enteroviruses of the family Picornaviridae. The structural changes observed in the empty IAPV particles include detachment of the VP4 minor capsid proteins from the inner face of the capsid and partial loss of the structure of the N-terminal arms of the VP2 capsid proteins. Unlike the case for many picornaviruses, the empty particles of IAPV are not expanded relative to the native virions and do not contain pores in their capsids that might serve as channels for genome release. Therefore, rearrangement of a unique region of the capsid is probably required for IAPV genome release.
IMPORTANCE Honeybee populations in Europe and North America are declining due to pressure from pathogens, including viruses. Israeli acute bee paralysis virus (IAPV), a member of the family Dicistroviridae, causes honeybee colony collapse disorder in the United States. The delivery of virus genomes into host cells is necessary for the initiation of infection. Here we present a structural cryo-electron microscopy analysis of IAPV particles induced to release their genomes. We show that genome release is not preceded by an expansion of IAPV virions as in the case of related picornaviruses that infect vertebrates. Furthermore, minor capsid proteins detach from the capsid upon genome release. The genome leaves behind empty particles that have compact protein shells.

Accession Number: WOS:000393883300022

PubMed ID: 27928006

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fuzik, Tibor	J-2684-2017	0000-0002-1190-0210
Pridal, Antonin	S-5171-2017	0000-0002-5798-6785
Plevka, Pavel	H-8661-2014	0000-0003-4215-3315

ISSN: 0022-538X

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Record 132 of 491

Title: An automated method to evaluate the enzyme kinetics of -glucosidases

Author(s): Klimes, P (Klimes, Pavel); Mazura, P (Mazura, Pavel); Turek, D (Turek, Dusan); Brzobohaty, B (Brzobohaty, Bretislav)

Source: PROTEIN SCIENCE **Volume:** 26 **Issue:** 2 **Pages:** 382-388 **DOI:** 10.1002/pro.3078 **Published:** FEB 2017

Abstract: Enzyme kinetic measurements are important for the characterization and engineering of biocatalysts, with applications in a wide range of research fields. The measurement of initial reaction velocity is usually slow and laborious, which motivated us to explore the possibilities for automating this process. Our model enzyme is the maize -glucosidase Zm-p60.1. Zm-p60.1 plays a significant role in plant growth and development by regulating levels of the active plant hormone cytokinin. Zm-p60.1 belongs to a wide group of hydrolytic enzymes. Members of this group hydrolyze several different types of glucosides, releasing glucose as a secondary product. Enzyme kinetic measurements using artificial substrates are well established, but burdensome and time-consuming. Thus, they are a suitable target for process automation. Simple optical methods for enzyme kinetic measurements using natural substrates are often impossible given the optical properties of the enzymatic reaction products. However, we have developed an automated method based on glucose detection, as glucose is released from all substrates of glucosidase reactions. The presented method can obtain 24 data points from up to 15 substrate concentrations to precisely describe the enzyme kinetics. The combination of an automated liquid handling process with assays that have been optimized for measuring the initial hydrolysis velocity of -glucosidases yields two distinct methods that are faster, cheaper, and more accurate than the established protocols.

Accession Number: WOS:000393960300021

PubMed ID: 27862518

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mazura, Pavel	D-7959-2012	

ISSN: 0961-8368
eISSN: 1469-896X

Record 133 of 491

Title: BAL31-NGS approach for identification of telomeres de novo in large genomes
Author(s): Peska, V (Peska, Vratislav); Sitova, Z (Sitova, Zdenka); Fajkus, P (Fajkus, Petr); Fajkus, J (Fajkus, Jiri)
Source: METHODS **Volume:** 114 **Pages:** 16-27 **DOI:** 10.1016/j.ymeth.2016.08.017 **Published:** FEB 1 2017
Abstract: This article describes a novel method to identify as yet undiscovered telomere sequences, which combines next generation sequencing (NGS) with BAL31 digestion of high molecular weight DNA. The method was applied to two groups of plants: i) dicots, genus Cestrum, and ii) monocots, Allium species (e.g. A. ursinum and A. cepa). Both groups consist of species with large genomes (tens of Gb) and a low number of chromosomes (2n =14-16), full of repeat elements. Both genera lack typical telomeric repeats and multiple studies have attempted to characterize alternative telomeric sequences. However, despite interesting hypotheses and suggestions of alternative candidate telomeres (retrotransposons, rDNA, satellite repeats) these studies have not resolved the question. In a novel approach based on the two most general features of eukaryotic telomeres, their repetitive character and sensitivity to BAL31 nuclease digestion, we have taken advantage of the capacity and current affordability of NGS in combination with the robustness of classical BAL31 nuclease digestion of chromosomal termini. While representative samples of most repeat elements were ensured by low-coverage (less than 5%) genomic shot-gun NGS, candidate telomeres were identified as under-represented sequences in BAL31-treated samples. (C) 2016 Elsevier Inc. All rights reserved.
Accession Number: WOS:000393251500003
PubMed ID: 27595912
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fajkus, Jiri	D-2499-2012	0000-0002-3112-1716
Peska, Vratislav		0000-0002-0526-2988

ISSN: 1046-2023
eISSN: 1095-9130

Record 134 of 491

Title: Fragmentation of Kr-N(+) clusters after electron impact ionization. Short-time dynamics simulations and approximate multi-scale treatment
Author(s): Janecek, I (Janecek, Ivan); Naar, P (Naar, Pavel); Stachon, M (Stachon, Martin); Gadea, FX (Gadea, Florent Xavier); Kalus, R (Kalus, Rene)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 4 **Pages:** 2778-2790 **DOI:** 10.1039/c6cp07479k **Published:** JAN 28 2017
Abstract: Post-ionization fragmentation of small ionic krypton clusters, Kr-N(+) (N = 3-13), has been investigated using a semiclassical non-adiabatic dynamics approach consisting of classical treatment of atomic nuclei and full quantum treatment of electrons, and an extended diatomics-in-molecules model including the spin-orbit coupling as well as leading three-body interaction corrections. Electronic quantum decoherence has also been considered via a simplified scheme proposed previously. The positive charge has been initially localized on a randomly selected atom in the form of a localized P-2(1/2) positive hole. It follows from the calculations that the data are not converged at timescales usually considered in dynamical calculations (t = 200 ps in this work) and that an extension to t approximate to 1 ms is needed. An approximate multi-scale treatment developed recently has been used to provide such an extension of the output of dynamical calculations. A qualitative agreement with available experimental data has been achieved, in particular, the experimental observation that the monomer fragment, Kr+, completely dominates has been reproduced. Interestingly, stabilized neutral dimer and trimer fragments have been observed in our calculations at non-negligible abundances despite extremely weak bonding in these species.
Accession Number: WOS:000394940400015
PubMed ID: 28067346
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kalus, Rene	O-6552-2017	0000-0002-6722-6640

ISSN: 1463-9076
eISSN: 1463-9084

Record 135 of 491

Title: Interface Tuning of Current-Induced Cooling in Molecular Circuits
Author(s): Foti, G (Foti, Giuseppe); Vazquez, H (Vazquez, Hector)
Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 121 **Issue:** 2 **Pages:** 1082-1088 **DOI:** 10.1021/acs.jpcc.6b11955 **Published:** JAN 19 2017
Abstract: We study the effect of the atomistic structure of metal-molecule contacts on the current-induced damping and excitation of vibrations in molecular circuits by means of first-principles calculations. We consider a carbene-based molecule bound to Au electrodes via three different tip terminations: a tetramer, a pyramid, and a chainlike structure. The change in the width and position of molecular levels associated with each of these metal-molecule structures under an applied voltage controls the heating and cooling processes. In blunt tips, where the electronic coupling between molecular and Au bulk states is strong, the cooling efficiency decreases as a function of bias which results in the heating of the most active vibrational modes. On the other hand, in chainlike structures where the coupling is weak, the cooling rate has a nonmonotonic behavior as a function of the applied bias and increases sharply beyond a certain voltage. This results in a current induced cooling at high bias. These findings open the way to the efficient removal of excess heat from the junction through control of the metal-molecule contact structures.
Accession Number: WOS:000392554000012
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922

ISSN: 1932-7447

Record 136 of 491

Title: Cryo-EM study of slow bee paralysis virus at low pH reveals iflavirus genome release mechanism
Author(s): Kalynych, S (Kalynych, Sergei); Fuzik, T (Fuzik, Tibor); Pridal, A (Pridal, Antonin); de Miranda, J (de Miranda, Joachim); Plevka, P (Plevka, Pavel)
Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA **Volume:** 114 **Issue:** 3 **Pages:** 598-603 **DOI:** 10.1073/pnas.1616562114 **Published:** JAN 17 2017
Abstract: Viruses from the family Iflaviridae are insect pathogens. Many of them, including slow bee paralysis virus (SBPV), cause lethal diseases in honeybees and bumblebees, resulting in agricultural losses. Iflaviruses have nonenveloped icosahedral virions containing single-stranded RNA genomes. However, their genome release mechanism is unknown. Here, we show that low pH promotes SBPV genome release, indicating that the virus may use endosomes to enter host cells. We used cryo-EM to study a heterogeneous population of SBPV virions at pH 5.5. We determined the structures of SBPV particles before and after genome release to resolutions of 3.3 and 3.4 angstrom, respectively. The capsids of SBPV virions in low pH are not expanded. Thus, SBPV does not appear to form "altered" particles with pores in their capsids before genome release, as is the case in many related picornaviruses. The egress of the genome from SBPV virions is associated with a loss of interpentamer contacts mediated by N-terminal arms of VP2 capsid proteins, which result in the expansion of the capsid. Pores that are 7 angstrom an diameter form around icosahedral threefold symmetry axes. We speculate that they serve as channels for the genome release. Our findings provide an atomic-level characterization of the genome release mechanism of iflaviruses.
Accession Number: WOS:000392095800054
PubMed ID: 28053231
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Pridal, Antonin	S-5171-2017	0000-0002-5798-6785
Fuzik, Tibor	J-2684-2017	0000-0002-1190-0210
Plevka, Pavel	H-8661-2014	0000-0003-4215-3315
Rodrigues de Miranda, Joachim		0000-0002-0335-0386

ISSN: 0027-8424

Record 137 of 491

Title: An efficient 2D B-11-B-11 solid-state NMR spectroscopy strategy for monitoring covalent self-assembly of boronic acid-derived compounds: the transformation and unique architecture of bortezomib molecules in the solid state

Author(s): Brus, J (Brus, J.); Czernek, J (Czernek, J.); Urbanova, M (Urbanova, M.); Kobera, L (Kobera, L.); Jegorov, A (Jegorov, A.)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 19 **Issue:** 1 **Pages:** 487-495 **DOI:** 10.1039/c6cp06555d **Published:** JAN 7 2017

Abstract: The difficulty in the prediction of the complicated solid-state structure of boronic acid derivatives, resulting from the complex pathway of reversible covalent interactions, represents a significant obstacle to the development of a new generation of advanced supramolecular systems such as covalent organic frameworks of efficient anticancer drugs. In this contribution, various 2D B-11-B-11 solid-state NMR correlation techniques supported by DFT calculations were explored to formulate a reliable tool for monitoring the covalent assembly of boronic acid residues in the solid state. This way, the self-condensation of bortezomib molecules was investigated, different local constitutions of boroxine motifs were unveiled, and the previously unreported boroxine structures of bortezomib polymorphs exhibiting secondary coordination were discovered and described in detail. The recorded B-11 NMR parameters responded sensitively to subtle changes in the local geometries, which were reliably interpreted and directly visualized by the DFT calculations. A uniform 2.6 angstrom distance in bortezomib B-11-B-11 spin pairs was conclusively identified by the through-space B-11-B-11 double-quantum (DQ) coherence build-up curves, whereas distinct 2D B-11-B-11 DQ correlation patterns revealed unique boroxine structures existing in the crystalline as well as amorphous state. The boroxine rings were found to be internally stabilized through the transformation of the trigonal boron sites toward tetrahedral geometry, as the secondary five-mmbered rings were formed. This way, the nature of bortezomib polymorphism is disclosed, and an efficient strategy for exploring the assembly of boronic acid derivatives in the solid state, for which no crystallographic data are available, is thus demonstrated.

Accession Number: WOS:000391725300051

PubMed ID: 27905605

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Brus, Jiri	G-3459-2014	
Czernek, Jiri	H-6708-2014	
Kobera, Libor	G-5237-2014	0000-0002-8826-948X
Urbanova, Martina	G-9793-2014	0000-0003-1316-6395

ISSN: 1463-9076

eISSN: 1463-9084

Record 138 of 491

Title: Spin-orbit torques in locally and globally noncentrosymmetric crystals: Antiferromagnets and ferromagnets

Author(s): Zelezny, J (Zelezny, J.); Gao, H (Gao, H.); Manchon, A (Manchon, Aurelien); Freimuth, F (Freimuth, Frank); Mokrousov, Y (Mokrousov, Yuriy); Zemen, J (Zemen, J.); Masek, J (Masek, J.); Sinova, J (Sinova, Jairo); Jungwirth, T (Jungwirth, T.)

Source: PHYSICAL REVIEW B **Volume:** 95 **Issue:** 1 **Article Number:** 014403 **DOI:** 10.1103/PhysRevB.95.014403 **Published:** JAN 5 2017

Abstract: One of the main obstacles that prevents practical applications of antiferromagnets is the difficulty of manipulating the magnetic order parameter. Recently, following the theoretical prediction [J.. Zelezny et al., Phys. Rev. Lett. 113, 157201 (2014)], the electrical switching of magnetic moments in an antiferromagnet was demonstrated [P. Wadley et al., Science 351, 587 (2016)]. The switching is due to the so-called spin-orbit torque, which has been extensively studied in ferromagnets. In this phenomena a nonequilibrium spin-polarization exchange coupled to the ordered local moments is induced by current, hence exerting a torque on the order parameter. Here we give a general systematic analysis of the symmetry of the spin-orbit torque in locally and globally noncentrosymmetric crystals. We study when the symmetry allows for a nonzero torque, when is the torque effective, and its dependence on the applied current direction and orientation of magnetic moments. For comparison, we consider both antiferromagnetic and ferromagnetic orders. In two representative model crystals we perform microscopic calculations of the spin-orbit torque to illustrate its symmetry properties and to highlight conditions under which the spin-orbit torque can be efficient for manipulating antiferromagnetic moments.

Accession Number: WOS:000391305800002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mokrousov, Yuriy	H-8517-2013	0000-0003-1072-2421
Zelezny, Jakub	G-5276-2014	0000-0001-9471-0078
Sinova, Jairo	G-9071-2014	0000-0002-9490-2333
Gao, Huawei	C-3325-2018	
Manchon, Aurelien	A-9355-2010	0000-0002-4768-293X
Zemen, Jan	H-1472-2014	0000-0002-7698-4945
Freimuth, Frank		0000-0001-6193-5991

ISSN: 2469-9950

eISSN: 2469-9969

Record 139 of 491

Title: Josephson-phase-controlled interplay between correlation effects and electron pairing in a three-terminal nanostructure

Author(s): Domanski, T (Domanski, T.); Zonda, M (Zonda, M.); Pokorny, V (Pokorny, V.); Gorski, G (Gorski, G.); Janis, V (Janis, V.); Novotny, T (Novotny, T.)

Source: PHYSICAL REVIEW B **Volume:** 95 **Issue:** 4 **Article Number:** 045104 **DOI:** 10.1103/PhysRevB.95.045104 **Published:** JAN 4 2017

Abstract: We study the subgap spectrum of the interacting single-level quantum dot coupled between two superconducting reservoirs, forming the Josephson-type circuit, and additionally hybridized with a metallic normal lead. This system allows for the phase-tunable interplay between the correlation effects and the proximity-induced electron pairing resulting in the singlet-doublet (0-pi) crossover and the phase-dependent Kondo effect. We investigate the spectral function, induced local pairing, Josephson supercurrent, and Andreev conductance in a wide range of system parameters by the numerically exact numerical renormalization group and quantum Monte Carlo calculations along with perturbative treatments in terms of the Coulomb repulsion and the hybridization term. Our results address especially the correlation effects reflected in dependencies of various quantities on the local Coulomb interaction strength as well as on the coupling to the normal lead. We quantitatively establish the phase-dependent Kondo temperature log T-K(phi) alpha cos(2)(phi/2) and show that it can be read off from the half-width of the zero-bias enhancement in the Andreev conductance in the doublet phase, which can be experimentally measured by the tunneling spectroscopy.

Accession Number: WOS:000391310500002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Janis, Vaclav	A-8379-2011	0000-0001-5959-6935
Novotny, Tomas	C-7392-2009	0000-0001-7014-4155
Zonda, Martin	M-9520-2015	0000-0002-8513-3392
Pokorny, Vladislav	G-5750-2014	0000-0002-8944-6417

ISSN: 2469-9950

eISSN: 2469-9969

Record 140 of 491

Title: Reference-free Identification of Phage DNA Using Signal Processing on Nanopore Data
Author(s): Kupkova, K (Kupkova, Kristyna); Sedlar, K (Sedlar, Karel); Provaznik, I (Provaznik, Ivo)
Book Group Author(s): IEEE
Source: 2017 IEEE 17TH INTERNATIONAL CONFERENCE ON BIOINFORMATICS AND BIOENGINEERING (BIBE) **Book Series:** IEEE International Conference on Bioinformatics and Bioengineering **Pages:** 101-105 **DOI:** 10.1109/BIBE.2017.00024 **Published:** 2017
Abstract: Nanopore sequencing has become an invaluable aid in small sequencing projects. Thanks to its compact size, the Oxford Nanopore MinION platform is often used in crisis situations, such as outbreaks of microbial infections, to determine the causes of the problem. As a platform that produces data in real-time, it requires bioinformatics techniques designed for fast data processing. In this paper, we demonstrate the possibility of the direct processing of nanopore current signals, the so-called squiggles, for fast reference-free identification of phage DNA. The proposed technique is based on the computation of Hjorth parameters and is suitable for fast visualization of the data, as well as for proper classification by many machine learning algorithms. The classification of the data also raises the possibility of applying adapted base calling algorithms for both groups separately, as phage and host DNA have different features.
Accession Number: WOS:000427878000017
Conference Title: 17th IEEE International Conference on Bioinformatics and Bioengineering (BIBE)
Conference Date: OCT 23-25, 2017
Conference Location: Herndon, VA
Conference Sponsors: IEEE, IEEE Comp Soc, Biol & Artificial Intelligence Soc
ISSN: 2471-7819
ISBN: 978-1-5386-1324-5

Record 141 of 491
Title: Documentation of Dark Areas of Large Historical Buildings by a Formation of Unmanned Aerial Vehicles using Model Predictive Control
Author(s): Saska, M (Saska, Martin); Kratky, V (Kratky, Vit); Spurny, V (Spurny, Vojtech); Baca, T (Baca, Tomas)
Book Group Author(s): IEEE
Source: 2017 22ND IEEE INTERNATIONAL CONFERENCE ON EMERGING TECHNOLOGIES AND FACTORY AUTOMATION (ETFA) **Book Series:** IEEE International Conference on Emerging Technologies and Factory Automation-ETFA **Published:** 2017
Abstract: A system designed for a unique multi-robot application of closely flying formations or Unmanned Aerial Vehicles (UANTS) in indoor areas is described in this paper. The proposed solution is aimed as a tool for historians and restorers working in large historical buildings such as churches to provide an access to areas that are difficult to reach by humans. In these objects, it is impossible to keep a large scaffolding for a long time due to regular services, which is necessary for studying a long-term influence of restorations works, and some parts or the churches were even not reached by people for decades and need to be inspected. To provide the same documentation and inspection techniques that are used by the experts in lower easily accessible parts of the buildings, we employ a formation of autonomous UAVs, where one of the robots is equipped by a visual sensor and the others by source of light, which provides the required flexibility for control or lightening.
The described system in its full complexity has been implemented with achieved robustness and reliability required by deployment in real missions. The technology demonstration has been provided with real UAVs in historical objects to help restorers and conservationists with achieved valuable results used in plans of restoration works. In these missions, UAVs were autonomously hovering at designated locations to be able to demonstrate usefulness of such robotic lightening approach.
Accession Number: WOS:000427812000089
Conference Title: 22nd IEEE International Conference on Emerging Technologies and Factory Automation (ETFA)
Conference Date: SEP 12-15, 2017
Conference Location: Limassol, CYPRUS
Conference Sponsors: IEEE, ABB, ies, Univ Cyprus, Dept Elect Comp Engn
ISSN: 1946-0740
ISBN: 978-1-5090-6505-9

Record 142 of 491
Title: Motion Planning with Motion Primitives for Industrial Bin Picking
Author(s): Vonasek, V (Vonasek, Vojtech); Vick, A (Vick, Axel); Saska, M (Saska, Martin)
Book Group Author(s): IEEE
Source: 2017 22ND IEEE INTERNATIONAL CONFERENCE ON EMERGING TECHNOLOGIES AND FACTORY AUTOMATION (ETFA) **Book Series:** IEEE International Conference on Emerging Technologies and Factory Automation-ETFA **Published:** 2017
Abstract: In the bin picking problem, the task is to automatically unload objects from a container using a robotic manipulator. The task is often approached by organizing the objects into a predictable pattern, e.g., a workpiece carrier, in order to simplify all integral subtasks like object recognition, motion planning and grasping. In such a case, motion planning can even be solved offline as it is ensured that the objects are always at the same positions at known times. However, there is a growing demand for non-structured bin picking, where the objects can be placed randomly in the bins. This arises from recent trends of transforming classical factories into smart production facilities allowing small lot sizes at the efficiency of mass production. The demand for fast and highly flexible handling and manipulation abilities of industrial robots requires to solve all the bin picking methods, including motion planning, online. In this paper, we propose a novel technique for fast sampling-based motion planning of robotic manipulators using motion primitives. Motion primitives are short trajectories that boost search of the configuration space and consequently speed up the planning phase. The proposed work has been verified in a simulation and on a prototype of a bin picking system.
Accession Number: WOS:000427812000194
Conference Title: 22nd IEEE International Conference on Emerging Technologies and Factory Automation (ETFA)
Conference Date: SEP 12-15, 2017
Conference Location: Limassol, CYPRUS
Conference Sponsors: IEEE, ABB, ies, Univ Cyprus, Dept Elect Comp Engn
ISSN: 1946-0740
ISBN: 978-1-5090-6505-9

Record 143 of 491
Title: SAT-Based Generation of Optimum Function Implementations with XOR Gates
Author(s): Fiser, P (Fiser, Petr); Halecek, I (Halecek, Ivo); Schmidt, J (Schmidt, Jan)
Edited by: Kubatova H; Novotny M; Skavhaug A
Source: 2017 EUROMICRO CONFERENCE ON DIGITAL SYSTEM DESIGN (DSD) **Pages:** 163-170 **DOI:** 10.1109/DSD.2017.74 **Published:** 2017
Abstract: This paper presents a method for generating optimum multi-level implementations of Boolean functions. It is based on Satisfiability (SAT) problem solving, while different SAT techniques are employed to reach different targets. The method is able to generate one, or enumerate all optimum implementations, while any technology constraints can be applied. Results for 4-input functions implemented by XOR-AND-Inverter-Graphs (XAIGs) with different XOR nodes costs are presented. Scalability and feasibility of the method is presented. Finally, an experimental evaluation of XAIG-based rewriting algorithm with optimum replacement circuits is presented and compared with the previous solution.
Accession Number: WOS:000427097100022
Conference Title: 20th Euromicro Conference on Digital System Design (DSD)
Conference Date: AUG 30-SEP 01, 2017
Conference Location: Vienna, AUSTRIA
Conference Sponsors: Univ Technol Vienna, Austrian Inst Technol, Austrian Comp Soc, OCG
ISBN: 978-1-5386-2146-2

Record 144 of 491
Title: SAT-based ATPG for Zero-Aliasing Compaction
Author(s): Hulle, R (Hulle, Robert); Fiser, P (Fiser, Petr); Schmidt, J (Schmidt, Jan)
Edited by: Kubatova H; Novotny M; Skavhaug A
Source: 2017 EUROMICRO CONFERENCE ON DIGITAL SYSTEM DESIGN (DSD) **Pages:** 307-314 **DOI:** 10.1109/DSD.2017.73 **Published:** 2017

Abstract: Aliasing in the test response compaction is an important source of fault coverage loss. Methods to avoid the aliasing generally require modification of the compactor to some extent. This can lead to a higher compactor complexity and consequently to higher area overhead, longer signal propagation delays, etc.
We propose a novel method, the Zero-aliasing ATPG (ZATPG), which is able to reduce the aliasing without need of designing new compactors. ZATPG works by augmenting the SAT-based ATPG process to constrain test pattern generation to produce no aliasing in the compactor. The method is general enough to be applicable to any compactor design.
We demonstrate our method on a LFSR-based MISR compactors, using the Single Stuck-At fault model. Our method is able to find a test with zero aliasing and complete fault coverage for smaller compactors than conventional, unguided ATPG. Thus, the area overhead of the compactor can be reduced, while the complete fault coverage is preserved.
Accession Number: WOS:000427097100043
Conference Title: 20th Euromicro Conference on Digital System Design (DSD)
Conference Date: AUG 30-SEP 01, 2017
Conference Location: Vienna, AUSTRIA
Conference Sponsors: Univ Technol Vienna, Austrian Inst Technol, Austrian Comp Soc, OCG
ISBN: 978-1-5386-2146-2

Record 145 of 491

Title: Line Rate Programmable Packet Processing in 100Gb Networks
Author(s): Benacek, P (Benacek, Pavel); Pus, V (Pus, Viktor); Korenek, J (Korenek, Jan); Kekely, M (Kekely, Michal)
Edited by: Santambrogio M; Gohringer D; Stroobandt D; Mentens N; Nurmi J
Source: 2017 27TH INTERNATIONAL CONFERENCE ON FIELD PROGRAMMABLE LOGIC AND APPLICATIONS (FPL) **Book Series:** International Conference on Field Programmable and Logic Applications **Published:** 2017
Abstract: The P4 language provides a way to describe a custom network packet processing behavior that involves header parsing, matching and assembling modified packets. Such abstraction represents a significant step towards removing the limitation of fixed-function networking devices. Our live demonstration shows a straightforward usage of an algorithm and tool that maps a P4 program to a general architecture of FPGA-based networking device. Network traffic is received, parsed, filtered and modified by the generated circuit at the full line rate of 100 Gbps Ethernet. The results of our ongoing joint research project NFV200 show that the FPGA technology can be used to improve network flexibility without the usual burden of tedious and error-prone HDL coding.
Accession Number: WOS:000426989400079
Conference Title: 27th International Conference on Field Programmable Logic and Applications (FPL)
Conference Date: SEP 04-08, 2017
Conference Location: Gent, BELGIUM
ISSN: 1946-1488
ISBN: 978-9-0903-0428-1

Record 146 of 491

Title: Multilinear analysis of Time-Resolved Laser-Induced Fluorescence Spectra of U(VI) containing natural water samples
Author(s): Visnak, J (Visnak, Jakub); Steudtner, R (Steudtner, Robin); Kassahun, A (Kassahun, Andrea); Hoth, N (Hoth, Nils)
Edited by: Aydin A; Sarpun IH; Tel E; Kaplan A; Demir B
Source: 3RD INTERNATIONAL CONFERENCE ON THEORETICAL AND EXPERIMENTAL STUDIES IN NUCLEAR APPLICATIONS AND TECHNOLOGY (TESNAT 2017) **Book Series:** EPJ Web of Conferences **Volume:** 154 **Article Number:** 01029 **DOI:** 10.1051/epjconf/201612802002 **Published:** 2017
Abstract: Natural waters' uranium level monitoring is of great importance for health and environmental protection. One possible detection method is the Time-Resolved Laser-Induced Fluorescence Spectroscopy (TRLFS), which offers the possibility to distinguish different uranium species. The analytical identification of aqueous uranium species in natural water samples is of distinct importance since individual species differ significantly in sorption properties and mobility in the environment. Samples originate from former uranium mine sites and have been provided by Wismut GmbH, Germany. They have been characterized by total elemental concentrations and TRLFS spectra. Uranium in the samples is supposed to be in form of uranyl(VI) complexes mostly with carbonate (CO32-)and bicarbonate (HCO3-) and to lesser extend with sulphate (SO42-), arsenate (AsO43-), hydroxo (OH-), nitrate (NO3-) and other ligands. Presence of alkaline earth metal dications (M = Ca2+, Mg2+, Sr2+) will cause most of uranyl to prefer ternary complex species, e.g. Mn(UO2)(CO3) 3(2n-4) (n.{1; 2}). From species quenching the luminescence, Cl- and Fe2+ should be mentioned. Measurement has been done under cryogenic conditions to increase the luminescence signal. Data analysis has been based on Singular Value Decomposition and monoexponential fit of corresponding loadings (for separate TRLFS spectra, the "Factor analysis of Time Series" (FATS) method) and Parallel Factor Analysis (PARAFAC, all data analysed simultaneously). From individual component spectra, excitation energies T-00, uranyl symmetric mode vibrational frequencies omega gs and excitation driven U-Oyl bond elongation. Delta R have been determined and compared with quasirelativistic (TD) DFT/B3LYP theoretical predictions to cross-check experimental data interpretation.
Accession Number: WOS:000426429000029
Conference Title: 3rd International Conference on Theoretical and Experimental Studies in Nuclear Applications and Technology (TESNAT)
Conference Date: MAY 10-12, 2017
Conference Location: Adana, TURKEY
ISSN: 2100-014X

Record 147 of 491

Title: Quantum algorithms for computational nuclear physics revisited, particular case of second quantized formulation
Author(s): Visnak, J (Visnak, Jakub); Vesely, P (Vesely, Petr)
Edited by: Aydin A; Sarpun IH; Tel E; Kaplan A; Demir B
Source: 3RD INTERNATIONAL CONFERENCE ON THEORETICAL AND EXPERIMENTAL STUDIES IN NUCLEAR APPLICATIONS AND TECHNOLOGY (TESNAT 2017) **Book Series:** EPJ Web of Conferences **Volume:** 154 **Article Number:** 01030 **DOI:** 10.1051/epjconf/201715401030 **Published:** 2017
Abstract: No core Full Configurational Interaction (NCFCI) calculations of Nuclear Bonding energy are resource demanding, in particular, computational time scales exponentially with the nucleon number A. In contrast to that, usage of quantum computers would allow an efficient (in polynomial time) NCFCI calculation and speed-up for other beyond-Mean-Field (correlation energy including) methods. To initiate feasibility studies of given quantum algorithms, we present an introduction to preliminary classicalcomputer simulation for the case of spherical nuclei (and He-4 in particular) within NCFCI with realistic chiral NNLO_opt potential.
Accession Number: WOS:000426429000030
Conference Title: 3rd International Conference on Theoretical and Experimental Studies in Nuclear Applications and Technology (TESNAT)
Conference Date: MAY 10-12, 2017
Conference Location: Adana, TURKEY
ISSN: 2100-014X

Record 148 of 491

Title: On Solution of the Dubins Touring Problem
Author(s): Faigl, J (Faigl, Jan); Vana, P (Vana, Petr); Saska, M (Saska, Martin); Baca, T (Baca, Tomas); Spurny, V (Spurny, Vojtech)
Book Group Author(s): IEEE
Source: 2017 EUROPEAN CONFERENCE ON MOBILE ROBOTS (ECMR) **Published:** 2017
Abstract: The Dubins traveling salesman problem (DTSP) combines the combinatorial optimization of the optimal sequence of waypoints to visit the required target locations with the continuous optimization to determine the optimal headings at the waypoints. Existing decoupled approaches to the DTSP are based on an independent solution of the sequencing part as the Euclidean TSP and finding the optimal headings of the waypoints in the sequence. In this work, we focus on the determination of the optimal headings in a given sequence of waypoints and formulate the problem as the Dubins touring problem (DTP). The DTP can be solved by a uniform sampling of possible headings; however, we propose a new informed sampling strategy to find approximate solution of the DTP. Based on the presented results, the proposed algorithm quickly converges to a high-quality solution, which is less than 0.1% from the optimum. Besides, the proposed approach also improves the solution of the DTSP, and its feasibility has been experimentally verified in a real practical deployment.
Accession Number: WOS:000426455100032
Conference Title: European Conference on Mobile Robots (ECMR)
Conference Date: SEP 06-08, 2017
Conference Location: Paris, FRANCE
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vana, Petr	K-5165-2017	0000-0003-2155-5788

ISBN: 978-1-5386-1096-1

Record 149 of 491

Title: Rotation moment invariants of vector fields

Author(s): Kostkova, J (Kostkova, Jitka)

Edited by: Hobza T

Source: SPSM 2017: STOCHASTIC AND PHYSICAL MONITORING SYSTEMS **Pages:** 49-58 **Published:** 2017

Abstract: Vector field images are a type of multidimensional data arising from many engineering areas. This type of images differs significantly from standard graylevel and color images in several aspects. Hence, there is a need for automatic processing of vector fields from application areas, developing special methods and algorithms for vector fields is of great importance. A common task in vector field analysis is the detection of various patterns of interest, such as sinks, vortices, saddle points, and others. The detection of these features is typically accomplished by template matching. The search algorithms must be primarily invariant to total rotation, where the action is applied not only on the spatial coordinates but also on the field values. Moment invariants of vector fields will be introduced. The superiority of orthogonal polynomials for construction of moments will be demonstrated. Their numerical stability will be shown to be higher than of the invariants published so far. The usefulness of invariants constructed from orthogonal moments will be demonstrated in a real world template matching application.

Accession Number: WOS:000425554500007

Conference Title: Stochastic and Physical Monitoring Systems Conference (SPMS 2017)

Conference Date: JUN 19-23, 2017

Conference Location: Dobrichovice, CZECH REPUBLIC

Conference Sponsors: Czech Tech Univ Prague, Dept Math, Grp Appl Math & Stochast

ISBN: 978-80-01-06338-5

Record 150 of 491

Title: Joint Stable Optical Frequency and Precise Time Transfer over 406 km of Shared Fiber Lines - Study

Author(s): Vojtech, J (Vojtech, Josef); Havlis, O (Havlis, Ondrej); Slapak, M (Slapak, Martin); Skoda, P (Skoda, Pavel); Smotlacha, V (Smotlacha, Vladimir); Velc, R (Velc, Radek); Munster, P (Munster, Petr); Kundrat, J (Kundrat, Jan); Altmann, M (Altmann, Michal); Radil, J (Radil, Jan); Altmannova, L (Altmannova, Lada); Vohnout, R (Vohnout, Rudolf); Hazlinsky, M (Hazlinsky, Michal); Horvath, T (Horvath, Tomas); Slavik, R (Slavik, Radan); Cizek, M (Cizek, Martin); Pravdova, L (Pravdova, Lenka); Rerucha, S (Rerucha, Simon); Hrabina, J (Hrabina, Jan); Cip, O (Cip, Ondrej)

Edited by: Herencsar N

Source: 2017 40TH INTERNATIONAL CONFERENCE ON TELECOMMUNICATIONS AND SIGNAL PROCESSING (TSP) **Pages:** 694-697 **Published:** 2017

Abstract: We present a preliminary study of bidirectional ultra-stable optical frequency and precise time transmission over 406 km long path in the telecom-grade fiber optic infrastructure of dense wavelength division multiplexing. The main challenge in this application is the need of bidirectional amplification to compensate for signal loss. Directional non-reciprocities of the time transfer are evaluated together with their uncertainties. Solutions are proposed to significantly limit the final uncertainty.

Accession Number: WOS:000425229000147

Conference Title: 40th International Conference on Telecommunications and Signal Processing (TSP)

Conference Date: JUL 05-07, 2017

Conference Location: Barcelona, SPAIN

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Rerucha, Simon	D-6924-2012	0000-0002-2026-5159
Cizek, Martin	I-7839-2012	0000-0001-6938-3423

ISBN: 978-1-5090-3982-1

Close

Web of Science
Page 4 (Records 151 -- 200)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 151 of 491

Title: Time Transfer Over 1900 km of DWDM Network

Author(s): Skoda, P (Skoda, Pavel); Radil, J (Radil, Jan); Vojtech, J (Vojtech, Josef); Smotlacha, V (Smotlacha, Vladimir); Munster, P (Munster, Petr); Zvanovec, S (Zvanovec, Stanislav)

Edited by: Herencsar N

Source: 2017 40TH INTERNATIONAL CONFERENCE ON TELECOMMUNICATIONS AND SIGNAL PROCESSING (TSP) **Pages:** 698-701 **Published:** 2017

Abstract: Since a dedicated optical infrastructure for atomic clock comparison is extremely expensive, we present our tests allowing sharing optical DWDM network. We expanded optical reach of our atomic clock comparison system and demonstrated the transfer of time information over 1900 km of DWDM system with other 8 neighbouring optical channels. NRENs have good potential to host time comparison applications for the academic community over long distances.

Accession Number: WOS:000425229000148

Conference Title: 40th International Conference on Telecommunications and Signal Processing (TSP)

Conference Date: JUL 05-07, 2017

Conference Location: Barcelona, SPAIN

ISBN: 978-1-5090-3982-1

Record 152 of 491

Title: Optical stabilization for time transfer infrastructure

Author(s): Vojtech, J (Vojtech, Josef); Altmann, M (Altmann, Michal); Skoda, P (Skoda, Pavel); Horvath, T (Horvath, Tomas); Slapak, M (Slapak, Martin); Smotlacha, V (Smotlacha, Vladimir); Havlis, O (Havlis, Ondrej); Munster, P (Munster, Petr); Radil, J (Radil, Jan); Kundrat, J (Kundrat, Jan); Altmannova, L (Altmannova, Lada); Velc, R (Velc, Radek); Hula, M (Hula, Miloslav); Vohnout, R (Vohnout, Rudolf)

Edited by: Novak E; Trolinger JD

Source: APPLIED OPTICAL METROLOGY II **Book Series:** Proceedings of SPIE **Volume:** 10373 **Article Number:** UNSP 1037310 **DOI:** 10.1117/12.2274815 **Published:** 2017

Abstract: In this paper, we propose and present verification of all-optical methods for stabilization of the end-to-end delay of an optical fiber link. These methods are verified for deployment within infrastructure for accurate time and stable frequency distribution, based on sharing of fibers with research and educational network carrying live data traffic. Methods range from path length control, through temperature conditioning method to transmit wavelength control. Attention is given to achieve continuous control for relatively broad range of delays. We summarize design rules for delay stabilization based on the character and the total delay jitter.

Accession Number: WOS:000425667000030

Conference Title: Conference on Applied Optical Metrology II

Conference Date: AUG 08-09, 2017

Conference Location: San Diego, CA

Conference Sponsors: SPIE

ISSN: 0277-786X

eISSN: 1996-756X

ISBN: 978-1-5106-1204-4; 978-1-5106-1203-7

Record 153 of 491

Title: Comparison of Interferometry Based and Polarization Based Sensing Systems for Use in Fiber Infrastructure Protection

Author(s): Munster, P (Munster, Petr); Horvath, T (Horvath, Tomas); Sysel, P (Sysel, Petr); Vojtech, J (Vojtech, Josef); Velc, R (Velc, Radek)

Book Group Author(s): IEEE

Source: 2017 INTERNATIONAL WORKSHOP ON FIBER OPTICS IN ACCESS NETWORK (FOAN) **Book Series:** International Workshop on Fiber Optics in Access Network **Published:** 2017

Abstract: Almost all data transmissions over long distances are transmitted through optical fibers. Fiber infrastructure is therefore very important and is necessary to protect it against fiber cuts caused e.g. by digging activity. Many network operators seeking appropriate solution for self protecting infrastructure system. We performed comparative measurement of the polarization based sensing system and the interferometry based sensing system to determine the sensitivity and accuracy of both systems. The results confirmed theoretical assumptions that both systems are suitable for strain measurement and the interferometry based sensing systems are more sensitive.

Accession Number: WOS:000425164500010

Conference Title: International Workshop on Fiber Optics in Access Network (FOAN)

Conference Date: NOV 06-08, 2017

Conference Location: Munich, GERMANY

ISSN: 2378-8488

ISBN: 978-1-5386-2413-5

Record 154 of 491

Title: A Videoconferencing System Based on WebRTC Technology

Author(s): Bestak, R (Bestak, Robert); Hlavacek, J (Hlavacek, Jiri)

Edited by: Gaj P; Kwiecien A; Sawicki M

Source: COMPUTER NETWORKS (CN 2017) **Book Series:** Communications in Computer and Information Science **Volume:** 718 **Pages:** 245-255 **DOI:** 10.1007/978-3-319-59767-6_20 **Published:** 2017

Abstract: Last years, videoconferencing systems are rapidly evolving and they are becoming more and more popular as a real time communication tool among users. A technology such as VoIP can be used in conjunction with desktop videoconferencing systems to enable low-cost face-to-face business meetings without a necessity to travel, especially for internationally oriented companies that have offices all around the word. In this paper, we focus on and discuss a videoconferencing platform based on the WebRTC technology. We analyze an impact on the multiplexing server's CPU load and memory requirements for different number of communicating users while taken into account different HW/SW configurations of end-point devices.

Accession Number: WOS:000425528200020

Conference Title: 24th International Conference on Computer Networks (CN)

Conference Date: JUN 20-23, 2017

Conference Location: Ladek Zdroj, POLAND

Conference Sponsors: IEEE Polish Sect, Silesian Univ Technol, Inst Informat

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bestak, Robert		0000-0003-3757-3921

ISSN: 1865-0929

eISSN: 1865-0937

ISBN: 978-3-319-59767-6

Record 155 of 491

Title: Dubins Orienteering Problem with Neighborhoods

Author(s): Penicka, R (Penicka, Robert); Faigl, J (Faigl, Jan); Vana, P (Vana, Petr); Saska, M (Saska, Martin)

Book Group Author(s): IEEE

Source: 2017 INTERNATIONAL CONFERENCE ON UNMANNED AIRCRAFT SYSTEMS (ICUAS'17) **Book Series:** International Conference on Unmanned Aircraft Systems **Pages:** 1555-1562 **Published:** 2017

Abstract: In this paper, we address the Dubins Orienteering Problem with Neighborhoods (DOPN) a novel problem derived from the regular Orienteering Problem (OP). In the OP, one tries to find a maximal reward collecting path through a subset of given target locations, each with associated reward, such that the resulting path length does not exceed the specified travel budget. The Dubins Orienteering Problem (DOP) requires the reward collecting path to satisfy the curvature-constrained model of the Dubins vehicle while reaching precise positions of the target locations. In the newly introduced DOPN, the resulting path also respects the curvature constrained Dubins vehicle as in the DOP; however, the reward can be collected within a close distant neighborhood of the target locations. The studied problem is inspired by data collection scenarios for an Unmanned Aerial Vehicle (UAV), that can be modeled as the Dubins vehicle. Furthermore, the DOPN is a useful problem formulation of data collection scenarios for a UAV with the limited travel budget due to battery discharge and in scenarios where the sensoric data can be collected from a proximity of each target location. The proposed solution of the DOPN is based on the Variable Neighborhood Search method, and the presented computational results in the OP benchmarks support feasibility of the proposed approach.

Accession Number: WOS:000425255200193

Conference Title: International Conference on Unmanned Aircraft Systems (ICUAS)

Conference Date: JUN 13-16, 2017

Conference Location: Miami, FL

Conference Sponsors: IEEE, CSS, IEEE Robot & Automat Soc, MCA

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vana, Petr	K-5165-2017	0000-0003-2155-5788
Faigl, Jan		0000-0002-6193-0792

ISSN: 2373-6720

ISBN: 978-1-5090-4494-8

Record 156 of 491

Title: Overlap detection for a genome assembly based on genomic signal processing

Author(s): Jugas, R (Jugas, Robin); Sedlar, K (Sedlar, Karel); Vitek, M (Vitek, Martin); Skutkova, H (Skutkova, Helena)

Edited by: Bamidis PD; Konstantinidis ST; Rodrigues PP

Source: 2017 IEEE 30TH INTERNATIONAL SYMPOSIUM ON COMPUTER-BASED MEDICAL SYSTEMS (CBMS) **Book Series:** IEEE International Symposium on Computer-Based Medical Systems **Pages:** 300-305 **DOI:** 10.1109/CBMS.2017.140 **Published:** 2017

Abstract: Although the genome sequences of most studied organisms, like human, E. coli, and others are already known, de novo genome sequencing remains popular as a majority of genomes remains unknown. Unfortunately, sequencing machines are able to read only short fragments of DNA. Therefore, one of the basic steps in reconstructing novel genomes lies in putting these pieces of DNA, called 'reads', together into complete genome sequences using a process known as genome assembly. Reads joining, however, requires efficient detection of their overlaps. This is commonly performed by comparing the particular characters (A, C, G, T) of the reads using string processing techniques. In this paper, we present an alternative way of detecting overlaps using genomic signal processing. Unlike string comparison, numerical phase signals reflect the complementarity of double stranded DNA making the signal ideal for effective strand independent overlap detection using covariance with high accuracy.

Accession Number: WOS:000424864800062

Conference Title: 30th IEEE International Symposium on Computer-Based Medical Systems (IEEE CBMS)

Conference Date: JUN 22-24, 2017

Conference Location: Aristotle Univ Thessaloniki, Thessaloniki, GREECE

Conference Sponsors: IEEE, Aristotle Univ Thessaloniki Res Comm, Univ Nottingham, ePBLnet, SmokeFreeBrain, LLM Care Hlth & Social Care Ecosystem, Open Knowledge Fdn Chapter Greece, MEDical Curriculum INnovat, Widening Access Virtual Educ Scenarios, Intelligent Parkinson Early Detect Guiding Novel Support Intervent, Ubiquitous iNteroperable Care Ageing People

Conference Host: Aristotle Univ Thessaloniki

ISSN: 2372-9198

ISBN: 978-1-5386-1710-6

Record 157 of 491

Title: Classifier fusion for VoIP attacks classification

Author(s): Safarik, J (Safarik, Jakub); Rezac, F (Rezac, Filip)

Edited by: Kadar I

Source: SIGNAL PROCESSING, SENSOR/INFORMATION FUSION, AND TARGET RECOGNITION XXVI **Book Series:** Proceedings of SPIE **Volume:** 10200 **Article Number:** UNSP 102001F **DOI:** 10.1117/12.2262744 **Published:** 2017

Abstract: SIP is one of the most successful protocols in the field of IP telephony communication. It establishes and manages VoIP calls. As the number of SIP implementation rises, we can expect a higher number of attacks on the communication system in the near future. This work aims at malicious SIP traffic classification. A number of various machine learning algorithms have been developed for attack classification. The paper presents a comparison of current research and the use of classifier fusion method leading to a potential decrease in classification error rate. Use of classifier combination makes a more robust solution without difficulties that may affect single algorithms. Different voting schemes, combination rules, and classifiers are discussed to improve the overall performance. All classifiers have been trained on real malicious traffic. The concept of traffic monitoring depends on the network of honeypot nodes. These honeypots run in several networks spread in different locations. Separation of honeypots allows us to gain an independent and trustworthy attack information.

Accession Number: WOS:000424391600040

Conference Title: Conference on Signal Processing, Sensor/Information Fusion, and Target Recognition XXVI

Conference Date: APR 10-12, 2017

Conference Location: Anaheim, CA

Conference Sponsors: SPIE

ISSN: 0277-786X

eISSN: 1996-756X

ISBN: 978-1-5106-0901-3; 978-1-5106-0902-0

Record 158 of 491

Title: SIMULATION OF THE APPLICATION LAYER IN NARROWBAND NETWORKS WITH CONDITIONAL DATA INJECTION XML SCHEME BASED ON UNIVERSAL DATA GENERATOR

Author(s): Vondrous, O (Vondrous, Ondrej); Macejko, P (Macejko, Peter); Kocur, Z (Kocur, Zbynek)

Source: ADVANCES IN ELECTRICAL AND ELECTRONIC ENGINEERING **Volume:** 15 **Issue:** 4 **Special Issue:** SI **Pages:** 639-647 **DOI:** 10.15598/aeee.v15i4.2454 **Published:** 2017

Abstract: In this article, we would like to deal with challenges and analysis approaches in the area of narrow band communication networks. Especially those networks which use TCP/IP protocol family. We also present a new universal data generator for OMNeT++ simulation environment. We created this generator to satisfy the evaluation, stress testing and benchmarking demands of more and more complex industrial and the Internet of Things networks. We also present the methods for evaluation and comparison of results obtained from simulated and real TCP/IP based networks in this article.

Accession Number: WOS:000424328700009

ISSN: 1336-1376

eISSN: 1804-3119

Record 159 of 491

Title: Spin-dependent electrical transport at finite temperatures from the first principles

Author(s): Wagneknecht, D (Wagneknecht, David); Carva, K (Carva, Karel); Turek, I (Turek, Ilja)

Edited by: Drouhin HJ; Wegrowe JE; Razeghi M; Jaffres H

Source: SPINTRONICS X **Book Series:** Proceedings of SPIE **Volume:** 10357 **Article Number:** UNSP 103572W **DOI:** 10.1117/12.2273315 **Published:** 2017

Abstract: The finite-temperature electrical transport properties depending on the spin are essential for spintronics research focused on developing devices that should operate not only in the conditions of low temperatures. In this study we present a theoretical approach incorporating both chemical and temperature-induced disorder within the coherent potential approximation and the tight-binding linear muffin-tin orbital method, and the linear response theory is used to obtain spin-resolved electrical conductivity. Both nonmagnetic and magnetic materials are studied from the first principles in a wide temperature range. It was found, with neglected magnetic disorder, that vertex corrections to the total conductivity and spin-flip contributions to the conductivity are small; therefore, the spin-resolved coherent conductivities can be used to describe spin-dependent electrical transport. The developed formalism is applied to pure nonmagnetic platinum and to ferromagnetic random Cu-Ni alloys. For the latter system, the spin polarization of the current is nearly constant in the examined temperature range.

Accession Number: WOS:000424081400023
Conference Title: 10th Spintronics Symposium
Conference Date: AUG 05-10, 2017
Conference Location: San Diego, CA
Conference Sponsors: SPIE

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Carva, Karel	A-3703-2008	0000-0002-2275-1986
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Wagenknecht, David		0000-0003-1927-9702

ISSN: 0277-786X
eISSN: 1996-756X
ISBN: 978-1-5106-1172-6; 978-1-5106-1171-9

Record 160 of 491

Title: A computational characterization of CO@C-60

Author(s): Slanina, Z (Slanina, Zdenek); Uhlik, F (Uhlik, Filip); Nagase, S (Nagase, Shigeru); Akasaka, T (Akasaka, Takeshi); Adamowicz, L (Adamowicz, Ludwik); Lu, X (Lu, Xing)

Source: FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES **Volume:** 25 **Issue:** 11 **Pages:** 624-629 **DOI:** 10.1080/1536383X.2017.1357548 **Published:** 2017

Abstract: The carbon monoxide encapsulation into C-60 is evaluated using the DFT and MP2 calculations. The CO encapsulation is attractive, yielding an energy gain of more than 12 kcal/mol. This substantial encapsulation energy should produce at the conditions used in the high-temperature and high-pressure synthesis (originally used for encapsulation of rare gases in fullerenes) an equilibrium CO@C-60 fraction of about 3.5% compared to the empty C-60. The computed IR and NMR spectra agree with the available observations for CO encapsulated into open-cage C-60 derivatives.

Accession Number: WOS:000423283900002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Uhlik, Filip	G-7395-2012	0000-0002-1628-2861

ISSN: 1536-383X
eISSN: 1536-4046

Record 161 of 491

Title: Towards Scalable Streaming to SAGE2 Video Walls

Author(s): Ubik, S (Ubik, Sven); Travnicek, Z (Travnicek, Zdenek)

Book Group Author(s): IEEE

Source: 2017 INTERNATIONAL CONFERENCE ON SYSTEMS, SIGNALS AND IMAGE PROCESSING (IWSSIP) **Book Series:** International Conference on Systems Signals and Image Processing **Published:** 2017

Abstract: Video walls are useful to display large visualizations. The SAGE2 web-based system allows easy programming of scalable visualization applications. However, it is not easy to stream high resolution video to SAGE2 powered video walls. We proposed several methods of high resolution video streaming to LCD walls, evaluated their performance and discuss their scalability and properties.

Accession Number: WOS:000419268300028
Conference Title: 24th International Conference on Systems, Signals and Image Processing (IWSSIP)
Conference Date: MAY 22-24, 2017
Conference Location: Poznan Univ Technology, Poznan, POLAND
Conference Sponsors: Poznan Univ Technol, Fac Elect & Telecommunicat, IEEE Poland Sect, EURASIP, Polish Acad Sci, Elect & Telecommunicat Comm, Signals Circuits & Elect Syst Sect
Conference Host: Poznan Univ Technology
ISSN: 2157-8672
ISBN: 978-1-5090-6344-4

Record 162 of 491

Title: Evolving Keras Architectures for Sensor Data Analysis

Author(s): Vidnerova, P (Vidnerova, Petra); Neruda, R (Neruda, Roman)

Edited by: Ganzha M; Maciaszek L; Paprzycki M

Source: PROCEEDINGS OF THE 2017 FEDERATED CONFERENCE ON COMPUTER SCIENCE AND INFORMATION SYSTEMS (FEDCSIS) **Book Series:** Federated Conference on Computer Science and Information Systems **Pages:** 109-112 **DOI:** 10.15439/2017F241 **Published:** 2017

Abstract: Deep neural networks enjoy high interest and have become the state-of-art methods in many fields of machine learning recently. Still, there is no easy way for a choice of network architecture. However, the choice of architecture can significantly influence the network performance.
This work is the first step towards an automatic architecture design. We propose a genetic algorithm for an optimization of a network architecture. The algorithm is inspired by and designed directly for the Keras library [1] that is one of the most common implementations of deep neural networks.
The target application is the prediction of air pollution based on sensor measurements. The proposed algorithm is evaluated on experiments on sensor data and compared to several fixed architectures and support vector regression.

Accession Number: WOS:000417412800015
Conference Title: Federated Conference on Computer Science and Information Systems (FedCSIS)
Conference Date: SEP 03-06, 2017
Conference Location: Prague, CZECH REPUBLIC
Conference Sponsors: PTI, IEEE

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Neruda, Roman	D-2442-2014	0000-0003-2364-5357
Vidnerova, Petra	G-2718-2014	0000-0003-3879-3459

ISSN: 2325-0348
ISBN: 978-8-3946-2537-5

Record 163 of 491

Title: Sensoric and Data Applications in National Research and Educational Networks

Author(s): Radil, J (Radil, Jan); Munster, P (Munster, Petr); Horvath, T (Horvath, Tomas); Havlis, O (Havlis, Ondrej); Skoda, P (Skoda, Pavel); Vojtech, J (Vojtech, Josef)
Book Group Author(s): IEEE
Source: 2017 CONFERENCE ON LASERS AND ELECTRO-OPTICS PACIFIC RIM (CLEO-PR) **Published:** 2017
Abstract: High speed optical data networks are ubiquitous today. Data transmissions are based on coherent detection principles and use multilevel phase modulations. But another area of new applications is for example fiber-optic sensing. Such non-data signals present new challenges when designing networks. National research and educational network are at the forefront of such new developments.
Accession Number: WOS:000417416900268
Conference Title: Conference on Lasers and Electro-Optics Pacific Rim (CLEO-PR)
Conference Date: JUL 31-AUG 04, 2017
Conference Location: Singapore, SINGAPORE
ISBN: 978-1-5090-6290-4

Record 164 of 491
Title: CONVOLUTIONAL NEURAL NETWORK FOR SPEAKER CHANGE DETECTION IN TELEPHONE SPEAKER DIARIZATION SYSTEM
Author(s): Hruz, M (Hruz, Marek); Zajic, Z (Zajic, Zbynek)
Book Group Author(s): IEEE
Source: 2017 IEEE INTERNATIONAL CONFERENCE ON ACOUSTICS, SPEECH AND SIGNAL PROCESSING (ICASSP) **Book Series:** International Conference on Acoustics Speech and Signal Processing ICASSP **Pages:** 4945-4949 **Published:** 2017
Abstract: The aim of this paper is to propose a speaker change detection technique based on Convolutional Neural Netvork (CNN) and evaluate its contribution to the performance of a speaker diarization system for telephone conversations. For the comparison we used an i-vector based speaker diarization system. The baseline speaker change detection uses Generalized Likelihood Ratio (GLR) metric. Experiments were conducted on the English part of the CallHome corpus. Our proposed CNN speaker change detection outperformed the GLR approach, reducing the Equal Error Rate relatively by 46 %. The final results on speaker diarization system indicate that the use of speaker change detection based on CNN is beneficial with relative improvement of diarization error rate by 28 %.
Accession Number: WOS:000414286205021
Conference Title: IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP)
Conference Date: MAR 05-09, 2017
Conference Location: New Orleans, LA
Conference Sponsors: IEEE, Inst Elect & Elect Engineers, Signal Proc Soc
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zajic, Zbynek		0000-0002-4153-6560

ISSN: 1520-6149
ISBN: 978-1-5090-4117-6

Record 165 of 491
Title: Defects and magnetic structure of CuMnSb
Author(s): Maca, F (Maca, Frantisek); Kudrnovsky, J (Kudrnovsky, Josef); Drchal, V (Drchal, Vaclav); Turek, I (Turek, Ilja)
Book Group Author(s): IOP
Source: 8TH JOINT EUROPEAN MAGNETIC SYMPOSIA (JEMS2016) **Book Series:** Journal of Physics Conference Series **Volume:** 903 **Article Number:** UNSP 012034 **DOI:** 10.1088/1742-6596/903/1/012034 **Published:** 2017
Abstract: Total energy calculations show that the antiferromagnetic (111) order is not the ground state for the ideal CuMnSb in contrast to the results of neutron diffraction experiments. The magnetic phases of the CuMnSb Heusler alloy were investigated with the aim to clarify the role of defects which exist in real samples (Mn-antisites on Cu, Mn-interstitials, and Cu-Mn swaps). The full-potential supercell approach and the Heisenberg model were used to find the magnetic structure of the CuMnSb with defects. Results of both types of calculations indicate that already low defect concentrations can promote the (111) antiferromagnetic structure.
Accession Number: WOS:000418558200034
Conference Title: 8th Joint European Magnetic Symposia (JEMS)
Conference Date: AUG 21-26, 2016
Conference Location: Glasgow, SCOTLAND
Conference Sponsors: EMA, Inst Phys
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Turek, Ilja	G-5553-2014	0000-0002-0604-6590

ISSN: 1742-6588

Record 166 of 491
Title: Design of Numerical Model for Thermoacoustic Devices Using OpenFOAM
Author(s): Tisovsky, T (Tisovsky, Tomas); Vit, T (Vit, Tomas)
Edited by: Zitek P; Klimko M; Newton K
Source: 36TH MEETING OF DEPARTMENTS OF FLUID MECHANICS AND THERMODYNAMICS **Book Series:** AIP Conference Proceedings **Volume:** 1889 **Article Number:** UNSP 020043-1 **DOI:** 10.1063/1.5004377 **Published:** 2017
Abstract: Thennoacoustic devices are increasingly popular especially because of their construction simplicity and the ability to easily convert waste heat into the form of usable energy. Aim of this paper is to introduce some of the effective procedures for creating a complex mathematical model of thennoacoustic devices in OpenFOAM.
Accession Number: WOS:000417391000043
Conference Title: 36th Meeting of Departments of Fluid Mechanics and Thermodynamics
Conference Date: JUN 13-15, 2017
Conference Location: Univ W Bohemia, Fac Mech Engn, Dept Power Syst Engn, Pilsen, CZECH REPUBLIC
Conference Sponsors: Doosan Skoda Power
Conference Host: Univ W Bohemia, Fac Mech Engn, Dept Power Syst Engn
ISSN: 0094-243X
ISBN: 978-0-7354-1572-0

Record 167 of 491
Title: MODELLING OF PHASE EQUILIBRIA IN THE Hf-V SYSTEM BELOW ROOM TEMPERATURE
Author(s): Vrest'al, J (Vrest'al, J.); Pavlu, J (Pavlu, J.); Wdowik, UD (Wdowik, U. D.); Sob, M (Sob, M.)
Source: JOURNAL OF MINING AND METALLURGY SECTION B-METALLURGY **Volume:** 53 **Issue:** 3 **Special Issue:** SI **Pages:** 239-247 **DOI:** 10.2298/JMMB170704032V **Published:** 2017
Abstract: W Phase transformation from orthorhombic HfV2 structure to cubic C15 Laves phase structure, which occurs during heating at about 114 K, is well known. In this contribution, a thermodynamic description of this phenomenon is provided supported by ab initio calculations. We utilize the third generation of thermodynamic database extending the Scientific Group Thermodata Europe (SGTE) unary data to zero Kelvin and demonstrate that it may be also applied to intermetallic phases. The data from a recent thermodynamic assessment of the Hf-V system (valid for temperatures above 298.15 K) were used and extended to zero Kelvin by the same method as it was used for unary data. Under the assumption of validity of harmonic approximation and electronic contribution to the heat capacity, the thermodynamics of C15 and orthorhombic phase were described. With the help of ab initio approach, we demonstrate that the HfV2 orthorhombic phase and C15 Laves phase are mechanically stable at 0 K and thanks to entropy stabilization they are in equilibrium with pure element phases in the temperature region of structural change.
Accession Number: WOS:000417723500011

ISSN: 1450-5339

Record 168 of 491

Title: SUMMER VENTILATION OF POULTRY HOUSE FOR CHICKEN FATTENING IN CFD MODELLING

Author(s): Cao, VD (Cao, Van Doan); Zajicek, M (Zajicek, Milan); Kic, P (Kic, Pavel)

Edited by: Malinovska L; Osadcuks V

Source: 16TH INTERNATIONAL SCIENTIFIC CONFERENCE: ENGINEERING FOR RURAL DEVELOPMENT **Book Series:** Engineering for Rural Development **Pages:** 461-466 **DOI:** 10.22616/ERDev2017.16.N091 **Published:** 2017

Abstract: The aim of this paper is a numerical analysis of ventilation of the buildings for broilers during summer. Ventilation is the most important operation for internal environment to achieve the best performance of chickens. At each stage of growth of the chicken an optimum performance zone exists, in which the chickens use the most of the energy from food for growth. The target temperature for the best performance of broilers during growth changes daily and therefore ventilation is necessary to be modified by a suitable method. During the fattening period the biological production and thermoregulatory ability of chickens change significantly. In summer at the end of the fattening period, the problem of making the internal environment is more significant. The fundamental problem will be solved by using mathematical simulation, and the speed of flow will be determined in the ventilated space. For the research in the airflow, for prediction of the expected speed and air temperatures CFD (computer fluid dynamics) software Fluent was used. The effects of the change of the geometry and outside temperature, the concentration of carbon oxides, ammonia and dust within the hall were also monitored. The examined results of the program Fluent in all variations of temperatures and geometry for the location of the ventilation systems will be compared and then the effects and aftermath within the climatic conditions will be evaluated.

Accession Number: WOS:000416378300068

Conference Title: 16th International Scientific Conference on Engineering for Rural Development

Conference Date: MAY 24-26, 2017

Conference Location: Latvia Univ Agr, Fac Engn, Jelgava, LATVIA

Conference Host: Latvia Univ Agr, Fac Engn

ISSN: 1691-3043

eISSN: 1691-5976

Record 169 of 491

Title: ClassBench-ng: Recasting ClassBench After a Decade of Network Evolution

Author(s): Matousek, J (Matousek, Jiri); Antichi, G (Antichi, Gianni); Lucansky, A (Lucansky, Adam); Moore, AW (Moore, Andrew W.); Korenek, J (Korenek, Jan)

Book Group Author(s): IEEE

Source: 2017 ACM/IEEE SYMPOSIUM ON ARCHITECTURES FOR NETWORKING AND COMMUNICATIONS SYSTEMS (ANCS) **Pages:** 204-216 **DOI:** 10.1109/ANCS.2017.33 **Published:** 2017

Abstract: Internet evolution is driven by a continuous stream of new applications and users driving the demand for services. To keep up with this, a never-stopping research has been transforming the Internet ecosystem over the time. Technological changes on both protocols (the uptake of IPv6) and network architectures (the adoption of Software Defined Networking) introduced new challenges for ASIC designers. In particular, IPv6 and OpenFlow increased the complexity of the rule matching problem, pushing researchers to build new packet classification algorithms capable to keep pace with a steady growth of link speed.
A lot of research effort identifies better lookup techniques capitalizing on the characteristics of rule sets. So far, the availability of small numbers of real rule sets and synthetic ones, generated with tools such as ClassBench, has boosted research in the IPv4 world. Starting from an analysis of rule sets taken from operational environments, we present ClassBench-ng, a new open source tool for the generation of synthetic IPv4, IPv6, and OpenFlow 1.0 rule sets exposing the same properties of real ones. We feel this tool can meet the requirements of nowadays researchers, boosting the rule matching research as ClassBench has done since ten years ago.

Accession Number: WOS:000417417600024

Conference Title: 13th ACM/IEEE Symposium on Architectures for Networking and Communications Systems (ANCS)

Conference Date: MAY 18-19, 2017

Conference Location: Beijing, PEOPLES R CHINA

Conference Sponsors: ACM, IEEE, SIGARCH, ACM SIGCOMM, IEEE Comp Soc, Huawei, ZTE Commun, Tsinghua Natl Lab

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Antichi, Gianni		0000-0002-6063-4975

ISBN: 978-1-5090-6386-4

Record 170 of 491

Title: Simultaneous transmission of the high-power phase sensitive OTDR, 100 Gbps dual polarisation QPSK, accurate time/frequency, and their mutual interferences

Author(s): Munster, P (Munster, P.); Radil, J (Radil, J.); Vojtech, J (Vojtech, J.); Havlis, O (Havlis, O.); Horvath, T (Horvath, T.); Smotlacha, V (Smotlacha, V); Skaljo, E (Skaljo, E.)

Edited by: Baldwin CS; Pickrell G; Du HH; Udd E; Benterou JJ; Wang A

Source: FIBER OPTIC SENSORS AND APPLICATIONS XIV **Book Series:** Proceedings of SPIE **Volume:** 10208 **Article Number:** UNSP 102080D **DOI:** 10.1117/12.2267259 **Published:** 2017

Abstract: Currently, fibre networks are only way how to satisfy the ever growing needs for more bandwidth. Thanks to that the optical fibre can be found almost anywhere and new applications and services can be transmitted through the networks. Accurate time transfer, ultra-stable frequency transfer and fibre-optic sensors networks have been rather common. High speed data transmission, time and frequency transmission, and fibre-optic sensors must share the common fibre-optic infrastructure because it would not be economically feasible to build separate fibre networks for long distances. Each system has individual transmission requirements and is prone to another type of interference. Data transmission systems based on DP-QPSK or DP-xQAM use digital signal processing for signal recovering but it cannot fully compensate signal degradation due to polarization dependent loss and nonlinear effects which are the most dominant sources of signal degradation. Accurate time signals are slow and often OOK modulated, therefore may experience the degrading effect of chromatic dispersion. Ultra-stable frequency signals are not modulated at all information transmitted is the frequency of photons and such signals are continuous wave, but they suffer from phase noise also environmentally introduced, e.g. by vibrations. For phase sensitive OTDR sensor systems the high power pulses are necessary to use which may cause interference with other signals. For this reason, parallel and simultaneous transmission in DWDM spectral grids of standard data, time, frequency, and sensing signals is rather new and unexplored area of research.

Accession Number: WOS:000417002800009

Conference Title: Conference on Fiber Optic Sensors and Applications XIV

Conference Date: APR 11-12, 2017

Conference Location: Anaheim, CA

Conference Sponsors: SPIE

ISSN: 0277-786X

eISSN: 1996-756X

ISBN: 978-1-5106-0918-1; 978-1-5106-0917-4

Record 171 of 491

Title: Modular system for measuring a speech quality in the IP telephony infrastructures using autonomous probes

Author(s): Rezac, F (Rezac, Filip); Safarik, J (Safarik, Jakub); Macura, L (Macura, Lukas); Rozhon, J (Rozhon, Jan); Gresak, E (Gresak, Erik)

Edited by: Hall RD; Blowers M; Williams J

Source: DISRUPTIVE TECHNOLOGIES IN SENSORS AND SENSOR SYSTEMS **Book Series:** Proceedings of SPIE **Volume:** 10206 **Article Number:** UNSP 1020604 **DOI:** 10.1117/12.2258219 **Published:** 2017

Abstract: The paper deals with a speech quality monitoring system using probes placed on the individual network nodes operating VoIP services. Information on speech quality is measured periodically and the results are then stored on the central server which provides visualization in a form of graph respecting a topology of the probes. Article provides overall description of the technology and algorithms used in the speech quality monitoring system and results achieved in this applied research are verified in real operation. Contribution of the work lies in a proposal of the new multi-agent system enabling speech quality monitoring and in own implementation and its verification in Czech academic network.

Accession Number: WOS:000416983600003
Conference Title: Conference on Disruptive Technologies in Sensors and Sensor Systems
Conference Date: APR 11-12, 2017
Conference Location: Anaheim, CA
Conference Sponsors: SPIE
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Rozhon, Jan		0000-0003-4768-6073
Safarik, Jakub		0000-0002-3360-2302

ISSN: 0277-786X
eISSN: 1996-756X
ISBN: 978-1-5106-0913-6; 978-1-5106-0914-3

Record 172 of 491
Title: Strong effect of the interaction potential cut-off on the crystallinity of films grown by simulations
Author(s): Matas, M (Matas, Martin); Houska, J (Houska, Jiri)
Source: MOLECULAR SIMULATION **Volume:** 43 **Issue:** 17 **Pages:** 1436-1441 **DOI:** 10.1080/08927022.2017.1319056 **Published:** 2017
Abstract: The paper deals with the methodology of film growth simulations using classical molecular dynamics and an empirical interaction potential. We focus on the effect of the cut-off distance (r(C)) of the short-range part of the potential. On the one hand, we find that r(C) does not affect the qualitative conclusions of the simulations and that its quantitative effect is in the logical direction (better crystallinity at higher r(C)). On the other hand, we show that the aforementioned quantitative effect is very strong, and clearly underestimated in the literature. The film crystallinity is affected by (non-)neglecting of as seemingly low energies as several meV per bond. The results are important for the design of growth simulations of crystalline films and for the correct interpretation of their results.
Accession Number: WOS:000416674800004
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houska, Jiri	B-9616-2016	0000-0002-4809-4128

ISSN: 0892-7022
eISSN: 1029-0435

Record 173 of 491
Title: AN INVESTIGATION OF MASS TRANSFER IN A VORTEX SHEDDING PAST SQUARE CYLINDER
Author(s): Korinek, T (Korinek, T.); Petrikova, M (Petrikova, M.)
Book Group Author(s): IT/ASCR
Source: ENGINEERING MECHANICS 2017 **Book Series:** Engineering Mechanics **Pages:** 482-485 **Published:** 2017
Abstract: This work investigates mass transfer in a vortex shedding past a square cylinder. The investigation is done by numerical simulations and an experiment on a hydrodynamic table. Turbulence is modeled by Large Eddy Simulation method. Investigated range of Reynolds numbers (Re) is Re = 6 600 - 20 000 for numerical simulations and Re = 1.000 - 2 000 for the experiment. Obtained results indicate influence of Re on a distribution of an additional fluid in flow, where the leading edge of the square cylinder had a significant effect to the mass transfer in the spanwise direction.
Accession Number: WOS:000411657600110
Conference Title: 23rd International Conference on Engineering Mechanics
Conference Date: MAY 15-18, 2017
Conference Location: Svratka, CZECH REPUBLIC
Conference Sponsors: Brno Univ Technol, Inst Solid Mech, Fac Mech Engn, Acad Sci Czech Repub, v v i Branch Brno, Inst Thermomechan, Assoc Eng Mech, Acad Sci Czech Republ v v i, Inst Theoret & Appl Mech, ZDAS, a s Zdar nad Sazavon, Czech Soc Mech, IFToMM Member Comm Czech Republ
ISSN: 1805-8248
ISBN: 978-80-214-5497-2

Record 174 of 491
Title: GUST ALLEVIATION OF NASA COMMON RESEARCH MODEL USING CFD
Author(s): Prachar, A (Prachar, A.); Hospodar, P (Hospodar, P.); Vrchota, P (Vrchota, P.)
Book Group Author(s): IT/ASCR
Source: ENGINEERING MECHANICS 2017 **Book Series:** Engineering Mechanics **Pages:** 798-801 **Published:** 2017
Abstract: This paper presents a CFD study of a typical commercial aircraft entering the gust. The NASA Common Research model of an airliner is used as the baseline configuration. The gust model is based on adding artificial gust velocities into the governing equations, this method is usually referred to as Disturbance Velocity Approach. A series of gusts is used to measure response of the aircraft and to establish dynamic gust model. The movable control surfaces are defined and their efficiency is assessed by the CFD using the mesh deformation technique in the unsteady simulation. Finally, the dynamic model based on both the gust data on one hand and on the control surfaces action on the other hand is used to prescribe movement of the control surfaces with the aim to alleviate the gust interaction. The required time response of the control surfaces is studied to clarify limits of this alleviation technique.
Accession Number: WOS:000411657600189
Conference Title: 23rd International Conference on Engineering Mechanics
Conference Date: MAY 15-18, 2017
Conference Location: Svratka, CZECH REPUBLIC
Conference Sponsors: Brno Univ Technol, Inst Solid Mech, Fac Mech Engn, Acad Sci Czech Repub, v v i Branch Brno, Inst Thermomechan, Assoc Eng Mech, Acad Sci Czech Republ v v i, Inst Theoret & Appl Mech, ZDAS, a s Zdar nad Sazavon, Czech Soc Mech, IFToMM Member Comm Czech Republ
ISSN: 1805-8248
ISBN: 978-80-214-5497-2

Record 175 of 491
Title: INFLUENCE OF CERAMIC FOAM PARAMETERS ON THE FRACTURE BEHAVIOUR UPON THE TENSILE TEST
Author(s): Sevecek, O (Sevecek, O.); Majer, Z (Majer, Z.); Kotoul, M (Kotoul, M.)
Book Group Author(s): IT/ASCR
Source: ENGINEERING MECHANICS 2017 **Book Series:** Engineering Mechanics **Pages:** 862-865 **Published:** 2017
Abstract: The contribution deals with numerical simulation of response of the open cell ceramic foam to tensile loading and attempts to predict experimental fracture-mechanics behaviour of the foams using numerical FE model composed of beam elements. Models of different structure irregularity (including regular one) are considered and generated using 3D Voronoi tessellation technique. Complete fracture of the model is simulated by iterative FE simulations where in each step, one strut with maximal tensile stress (higher than the material tensile strength) is removed until complete separation of the model in two parts. Critical forces, leading to complete breakage of the foam structure, together with final fracture "surfaces", are investigated and compared for both regular and irregular structures. It is shown that the regular foam structure, composed of Kelvin cells, exhibit generally 10 - 20 % higher fracture resistance than the irregular foam structures and also that structures with smaller cells should be more fracture resistant than the structures with bigger cells.
Accession Number: WOS:000411657600205
Conference Title: 23rd International Conference on Engineering Mechanics
Conference Date: MAY 15-18, 2017
Conference Location: Svratka, CZECH REPUBLIC
Conference Sponsors: Brno Univ Technol, Inst Solid Mech, Fac Mech Engn, Acad Sci Czech Repub, v v i Branch Brno, Inst Thermomechan, Assoc Eng Mech, Acad Sci Czech Republ v v i, Inst Theoret & Appl Mech, ZDAS, a s Zdar nad Sazavon, Czech Soc Mech, IFToMM Member Comm Czech Republ

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sevecek, Oldrich	F-8238-2013	0000-0003-3442-2650

ISSN: 1805-8248

ISBN: 978-80-214-5497-2

Record 176 of 491

Title: Computing Maxmin Strategies in Extensive-form Zero-sum Games with Imperfect Recall

Author(s): Bosansky, B (Bosansky, Branislav); Cermak, J (Cermak, Jiri); Horak, K (Horak, Karel); Pechoucek, M (Pechoucek, Michal)

Edited by: VanDenHerik J; Rocha AP; Filipe J

Source: ICAART: PROCEEDINGS OF THE 9TH INTERNATIONAL CONFERENCE ON AGENTS AND ARTIFICIAL INTELLIGENCE, VOL 2 **Pages:** 63-74 **DOI:** 10.5220/0006121200630074 **Published:** 2017

Abstract: Extensive-form games with imperfect recall are an important game-theoretic model that allows a compact representation of strategies in dynamic strategic interactions. Practical use of imperfect recall games is limited due to negative theoretical results: a Nash equilibrium does not have to exist, computing maxmin strategies is NP-hard, and they may require irrational numbers. We present the first algorithm for approximating maxmin strategies in two-player zero-sum imperfect recall games without absentmindedness. We modify the well-known sequence-form linear program to model strategies in imperfect recall games resulting in a bilinear program and use a recent technique to approximate the bilinear terms. Our main algorithm is a branch-and-bound search that provably reaches the desired approximation after an exponential number of steps in the size of the game. Experimental evaluation shows that the proposed algorithm can approximate maxmin strategies of randomly generated imperfect recall games of sizes beyond toy-problems within few minutes.

Accession Number: WOS:000413244200006

Conference Title: 9th International Conference on Agents and Artificial Intelligence (ICAART)

Conference Date: FEB 24-26, 2017

Conference Location: Porto, PORTUGAL

ISBN: 978-989-758-220-2

Record 177 of 491

Title: Quantum-mechanical study of tensorial elastic and high-temperature thermodynamic properties of grain boundary states in superalloy-phase Ni3Al

Author(s): Friak, M (Friak, Martin); Vsianska, M (Vsianska, Monika); Holec, D (Holec, David); Sob, M (Sob, Mojmir)

Book Group Author(s): IOP

Source: 38TH RISO INTERNATIONAL SYMPOSIUM ON MATERIALS SCIENCE **Book Series:** IOP Conference Series-Materials Science and Engineering **Volume:** 219 **Article Number:** UNSP 012019 **DOI:** 10.1088/1757-899X/219/1/012019 **Published:** 2017

Abstract: Grain boundaries (GBs), the most important defects in solids and their properties are crucial for many materials properties including (in-) stability. Quantum-mechanical methods can reliably compute properties of GBs and we use them to analyze (tensorial) anisotropic elastic properties of interface states associated with GBs in one of the most important intermetallic compounds for industrial applications, Ni3Al. Selecting the Sigma 5(210) GBs as a case study because of its significant extra volume, we address the mechanical stability of the GB interface states by checking elasticity-based Born stability criteria. One critically important elastic constant, C-55, is found nearly three times smaller at the GB compared with the bulk, contributing thus to the reduction of the mechanical stability of Ni3Al polycrystals. Next, comparing properties of Sigma 5(210) GB state which is fully relaxed with those of a Sigma 5(210) GB state when the supercell dimensions are kept equal to those in the bulk we conclude that lateral relaxations have only marginal impact on the studied properties. Having the complete elastic tensor of Sigma 5(210) GB states we combine Green's-function based homogenization techniques and an approximative approach to the Debye model to compare thermodynamic properties of a perfect Ni3Al bulk and the Sigma 5(210) GB states. In particular, significant reduction of the melting temperature (to 79-81% of the bulk value) is predicted for nanometer-size grains.

Accession Number: WOS:000409355600019

Conference Title: 38th Riso International Symposium on Materials Science

Conference Date: SEP 04-08, 2017

Conference Location: Riso, DENMARK

ISSN: 1757-8981

Record 178 of 491

Title: Bryoerythrophyllum duellii Blockeel (Bryophyta: Pottiaceae), a new moss species from Greece and Cyprus, and its molecular affinities

Author(s): Blockeel, TL (Blockeel, Tom L.); Kucera, J (Kucera, Jan); Fedosov, VE (Fedosov, Vladimir E.)

Source: JOURNAL OF BRYOLOGY **Volume:** 39 **Issue:** 3 **Pages:** 247-254 **DOI:** 10.1080/03736687.2017.1317903 **Published:** 2017

Abstract: A moss first collected on Crete by Prof. Ruprecht Dull in 1976 but never satisfactorily identified is described as a new species, Bryoerythrophyllum duellii. It is known from five localities in Greece and Cyprus. It belongs to the B. recurvirostrum group, and its status as a distinct taxon is supported by molecular data. The molecular relationships of the genus Bryoerythrophyllum are discussed, and they suggest that the genus is monophyletic only if Erythrophyllopsis, Mironia and Saitobryum are included. The B. recurvirostrum and B. wallichii groups apparently form a young complex of taxa that are not very diverse molecularly, but sometimes have a distinctive morphology. Bryoerythrophyllum duellii is one of several lineages within this complex that may have experienced a longer period of reproductive isolation leading to the fixation of distinctive morphological and molecular features.

Accession Number: WOS:000407971400004

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fedosov, Vladimir	P-7066-2014	
Kucera, Jan	B-3633-2009	0000-0002-0230-5997

ISSN: 0373-6687

eISSN: 1743-2820

Record 179 of 491

Title: Simultaneous transmission of standard data, precise time, stable frequency and sensing signals and their possible interaction

Author(s): Munster, P (Munster, P.); Horvath, T (Horvath, T.); Havlis, O (Havlis, O.); Vojtech, J (Vojtech, J.); Radil, J (Radil, J.); Vele, R (Vele, R.); Skaljo, E (Skaljo, E.)

Edited by: Baldini F; Homola J; Lieberman RA

Source: OPTICAL SENSORS 2017 **Book Series:** Proceedings of SPIE **Volume:** 10231 **Article Number:** UNSP 102312A **DOI:** 10.1117/12.2266240 **Published:** 2017

Abstract: Since optical fibre is a standard medium for all current and new networks, these optical networks offer possibility for connecting new applications over long distances almost to anywhere. However with increasing number of applications, the large number of dedicated fibres will be necessary. This constitution is quite unpractical in terms of costs, however since wavelength division multiplexing enables transmission of multiple different signals over one fibre it is more than suitable to use this technology for cost reduction and network efficiency increase. Wavelength division multiplexing technology is common in data networks where parameters of all signals may be optimized (especially maximum optical power launched into the fibre) for simultaneous transmission. In case of non-data applications the situation is more difficult because each application is connected by different type of signal and with its own requirements for transmission parameters. Hence it is necessary to evaluate possible interactions before field deployment. In this paper we deal with possible interaction of a coherent 100 Gb/s dual polarisation QPSK data signal with new applications like accurate time and stable frequency transmission and high-power pulse signal used for distributed sensing. In laboratory setup we performed a measurement with a standard G.652D single mode optical fibre and also with G.655 fibre which can also be found in some networks and may be source of more nonlinear interactions. All signals were transmitted in a grid with 100GHz spacing according to ITU standard. Results confirmed our assumptions that 100GHz spacing is not large enough and also that G.655 optical fibre is prone to more non-linear interactions.

Accession Number: WOS:000407114800059

Conference Title: Conference on Optical Sensors

Conference Date: APR 24-27, 2017

Conference Location: Prague, CZECH REPUBLIC

Conference Sponsors: SPIE

ISSN: 0277-786X

ISBN: 978-1-5106-0963-1; 978-1-5106-0964-8

Record 180 of 491

Title: Particle dynamics and pair production in tightly focused standing wave

Author(s): Jirka, M (Jirka, M.); Klimo, O (Klimo, O.); Vranic, M (Vranic, M.); Weber, S (Weber, S.); Korn, G (Korn, G.)

Edited by: Korn G; Silva LO

Source: RESEARCH USING EXTREME LIGHT: ENTERING NEW FRONTIERS WITH PETAWATT-CLASS LASERS III **Book Series:** Proceedings of SPIE **Volume:** 10241 **Article Number:** UNSP 1024112 **DOI:** 10.1117/12.2271963 **Published:** 2017

Abstract: With the advent of 10 PW laser facilities, new regimes of laser-matter interaction are opening since effects of quantum electrodynamics, such as electron-positron pair production and cascade development, start to be important. The dynamics of light charged particles, such as electrons and positrons, is affected by the radiation reaction force. This effect can strongly influence the interaction of intense laser pulses with matter since it lowers the energy of emitting particles and transforms their energy to the gamma radiation. Consequently, electron positron pairs can be generated via Breit-Wheeler process. To study this new regime of interaction, numerical simulations are required. With their help it is possible to predict and study quantum effects which may occur in future experiments at modern laser facilities.
In this work we present results of electron interaction with an intense standing wave formed by two colliding laser pulses. Due to the necessity to achieve ultra intense laser field, the laser beam has to be focused to a similar to mu m-diameter spot. Since the paraxial approximation is not valid for tight focusing, the appropriate model describing the tightly focused laser beam has to be employed. In tightly focused laser beam the longitudinal component of the electromagnetic field becomes significant and together with the ponderomotive force they affect the dynamics of interacting electrons and also newly generated Breit-Wheeler electron-positron pairs. Using the Particle-In-Cell code we study electron dynamics, gamma radiation and pair production in such a configuration for linear polarization and different types of targets.

Accession Number: WOS:000406963300008

Conference Title: Conference on Research Using Extreme Light - Entering New Frontiers with Petawatt-Class Lasers III

Conference Date: APR 24-26, 2017

Conference Location: Prague, CZECH REPUBLIC

Conference Sponsors: SPIE

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Jirka, Martin	H-4152-2014	0000-0003-4457-4471
Vranic, Marija	K-6631-2015	0000-0003-3764-0645

ISSN: 0277-786X

ISBN: 978-1-5106-0983-9; 978-1-5106-0984-6

Record 181 of 491

Title: Experience with Optical Infrastructure for Time and Frequency Transfer

Author(s): Smotlacha, V (Smotlacha, Vladimir); Vojtech, J (Vojtech, Josef)

Book Group Author(s): INST NAVIGAT

Source: PROCEEDINGS OF THE 48TH ANNUAL PRECISE TIME AND TIME INTERVAL SYSTEMS AND APPLICATIONS MEETING **Book Series:** Annual Precise Time and Time Interval Systems and Applications Meeting **Pages:** 299-305 **Published:** 2017

Abstract: This paper describes the advanced version of the TF-infrastructure that utilizes links and other resources of Czech academic network CESNET2. Currently (2017), the total fiber length in the TF-infrastructure is over 1600 km of which 1100 km are in routine operation and the rest can be used for experiments. The DWDM (Dense Wavelength Division Multiplexing) technology is deployed on majority of the optical fibers and allows to share them with multiple date channels up to 200 Gb/s.

Accession Number: WOS:000404839300033

Conference Title: 48th Annual Precise Time and Time Interval Systems and Applications Meeting

Conference Date: JAN 30-FEB 01, 2017

Conference Location: Monterey, CA

Conference Sponsors: Inst Navigat

ISSN: 2333-2085

Record 182 of 491

Title: Large-scale cortico-subcortical functional networks in focal epilepsies: The role of the basal ganglia

Author(s): Vytvarova, E (Vytvarova, Eva); Marecek, R (Marecek, Radek); Fousek, J (Fousek, Jan); Strycek, O (Strycek, Ondrej); Rektor, I (Rektor, Ivan)

Source: NEUROIMAGE-CLINICAL **Volume:** 14 **Pages:** 28-36 **DOI:** 10.1016/j.nicl.2016.12.014 **Published:** 2017

Abstract: Objectives: The aimwas to describe the contribution of basal ganglia (BG) thalamo-cortical circuitry to thewholebrain functional connectivity in focal epilepsies.
Methods: Interictal resting-state fMRI recordings were acquired in 46 persons with focal epilepsies. Of these 46, 22 had temporal lobe epilepsy: 9 left temporal (LTLE), 13 right temporal (RTLE); 15 had frontal lobe epilepsy (FLE); and 9 had parietal/ occipital lobe epilepsy (POLE). There were 20 healthy controls. The completeweighted networkwas analyzed based on correlation matrices of 90 and 194 regions. The network topologywas quantified on a global and regional level by measures based on graph theory, and connection-level changes were analyzed by the partial least square method.
Results: In all patient groups except RTLE, the shift of the functional network topology away from random was observed (normalized clustering coefficient and characteristic path length were higher in patient groups than in controls). Links contributing to this change were found in the cortico-subcortical connections. Weak connections (low correlations) consistently contributed to thismodification of the network. The importance of regions changed: decreases in the subcortical areas and both decreases and increases in the cortical areas were observed in node strength, clustering coefficient and eigenvector centrality in patient groups when compared to controls. Node strength decreases of the basal ganglia, i.e. the putamen, caudate, and pallidum, were displayed in LTLE, FLE, and POLE. The connectivity within the basal ganglia-thalamus circuitry was not disturbed; the disturbance concerned the connectivity between the circuitry and the cortex.
Significance: Focal epilepsies affect large-scale brain networks beyond the epileptogenic zones. Cortico-subcortical functional connectivity disturbance was displayed in LTLE, FLE, and POLE. Significant changes in the restingstate functional connectivity between cortical and subcortical structures suggest an important role of the BG and thalamus in focal epilepsies. (C) 2017 The Authors. Published by Elsevier Inc.

Accession Number: WOS:000405984300003

PubMed ID: 28123951

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fousek, Jan		0000-0002-8371-2956

ISSN: 2213-1582

Record 183 of 491

Title: Deep data analysis in gigabit passive optical networks

Author(s): Horvath, T (Horvath, Tomas); Krkos, R (Krkos, Radko); Dubravec, L (Dubravec, Lunos)

Source: OPTICA APPLICATA **Volume:** 47 **Issue:** 1 **Pages:** 157-170 **DOI:** 10.5277/oa170114 **Published:** 2017

Abstract: This paper focuses on practical aspects of gigabit passive optical networks (GPON) diagnostics during deployment, for root-cause analysis and for research purposes. While GPON signalling analysis is already quite commonly used for diagnostics, the aim of this work is a holistic approach, including both signalling and user plane (payload) analysis. User plane analysis, especially if targeted at payload Ethernet, IP and transport layers, enables detection of additional group of problems that could limit or even prevent GPON internetworking and thus degrade the user perceived service quality. Integrated signalling and payload analysis is also interesting from the research point of view, leading to the ability to study equipment idiosyncrasies that would be hard to detect otherwise and it is also one of the enablers of equipment security verification. The mentioned theories were tested during a practical diagnostic session on a real GPON network deployment and this paper presents the findings.

Accession Number: WOS:000404196600015

ISSN: 0078-5466

eISSN: 1899-7015

Record 184 of 491

Title: The under-pressure behaviour of mechanical, electronic and optical properties of calcium titanate and its ground state thermoelectric response

Author(s): Noor, NA (Noor, N. A.); Alay-e-Abbas, SM (Alay-e-Abbas, S. M.); Hassan, M (Hassan, M.); Mahmood, I (Mahmood, I.); Alahmed, ZA (Alahmed, Z. A.); Reshak, AH (Reshak, A. H.)

Source: PHILOSOPHICAL MAGAZINE **Volume:** 97 **Issue:** 22 **Pages:** 1884-1901 **DOI:** 10.1080/14786435.2017.1320440 **Part:** A **Published:** 2017

Abstract: In this study, the elastic, electronic, optical and thermoelectric properties of CaTiO3 perovskite oxidehave been investigated using first-principles calculations. The generalised gradient approximation (GGA) has been employed for evaluating structural and elastic properties, while the modified Becke Johnson functional is used for studying the optical response of this compound. In addition to ground state physical properties, we also investigate the effects of pressure (0, 30, 60, 90 and 120 GPa) on the electronic structure of CaTiO3. The application of pressure from 0 to 90 GPa shows that the indirect band gap (-M) of CaTiO3 increases with increasing pressure and at 120 GPa it spontaneously decreases transforming cubic CaTiO3 to a direct (-) band gap material. The complex dielectric function and some optical parameters are also investigated under the application of pressures. All the calculated optical properties have been found to exhibit a shift to the higher energies with the increase of applied pressure suggesting potential optoelectronic device applications of CaTiO3. The thermoelectric properties of CaTiO3 have been computed at 0 GPa in terms of electrical conductivity, thermal conductivity and Seebeck coefficient.

Accession Number: WOS:000403712700003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363
Alahmed, Zeyad	F-1683-2013	0000-0001-7304-8118

ISSN: 1478-6435

eISSN: 1478-6443

Record 185 of 491

Title: Are XORs in Logic Synthesis Really Necessary?

Author(s): Halecek, I (Halecek, Ivo); Fiser, P (Fiser, Petr); Schmidt, J (Schmidt, Jan)

Edited by: Dietrich M; Novak O

Source: 2017 20TH IEEE INTERNATIONAL SYMPOSIUM ON DESIGN AND DIAGNOSTICS OF ELECTRONIC CIRCUIT & SYSTEMS (DDECS) **Book Series:** IEEE International Symposium on Design and Diagnostics of Electronic Circuits & Systems **Pages:** 134-139 **Published:** 2017

Abstract: This paper follows recent research on insufficient synthesis performance for XOR-intensive circuits, and introduces a novel logic representation with a native support of XOR gates, the XOR-AND-Inverter Graphs (XAIGs). A rewriting algorithm over XAIG has been implemented in the logic synthesis and optimization package ABC, as the first step towards a complete synthesis process. The results show that XAIG based rewriting can help to discover XORs and improves the area of a mapped network in some cases.

Accession Number: WOS:000403405200025

Conference Title: 20th IEEE International Symposium on Design and Diagnostics of Electronic Circuits and Systems (DDECS)

Conference Date: APR 19-21, 2017

Conference Location: Dresden, GERMANY

Conference Sponsors: IEEE, IEEE Comp Soc, Fraunhofer IIS, Cadence, BOSCH

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fiser, Petr	P-6744-2014	0000-0001-5306-6343

ISSN: 2334-3133

ISBN: 978-1-5386-0472-4

Record 186 of 491

Title: A Novel Architecture for LZS S Compression of Configuration Bitstreams Within FPGA

Author(s): Isa, R (Isa, Radek); Matousek, J (Matousek, Jiri)

Edited by: Dietrich M; Novak O

Source: 2017 20TH IEEE INTERNATIONAL SYMPOSIUM ON DESIGN AND DIAGNOSTICS OF ELECTRONIC CIRCUIT & SYSTEMS (DDECS) **Book Series:** IEEE International Symposium on Design and Diagnostics of Electronic Circuits & Systems **Pages:** 171-176 **Published:** 2017

Abstract: Partial run-time reconfigurability of current FPGAs has been shown to be beneficial in many application domains. However, utilization of this feature is limited by the time it takes to reconfigure a selected part of an FPGA. This is commonly addressed by compression of a configuration bitstream, often using LZSS algorithm. To allow speeding up the reconfiguration also in self-adaptive architectures, bitstream compression has to be done within FPGA. Therefore, this paper presents a novel architecture of an LZSS compression engine that is able to achieve very low resource utilization or throughput several times higher than similar architectures, while keeping the other parameter as well as compression ratio at acceptable level. The presented architecture is generic, thus the user can tune the input token size and the size of buffers to achieve desired characteristics. The paper also includes an evaluation of a trade-off among the size of input token, the size of buffers utilized in LZSS algorithm, and a compression ratio for several configuration bitstreams. This evaluation can help the user to select the right set of parameters for the architecture.

Accession Number: WOS:000403405200031

Conference Title: 20th IEEE International Symposium on Design and Diagnostics of Electronic Circuits and Systems (DDECS)

Conference Date: APR 19-21, 2017

Conference Location: Dresden, GERMANY

Conference Sponsors: IEEE, IEEE Comp Soc, Fraunhofer IIS, Cadence, BOSCH

ISSN: 2334-3133

ISBN: 978-1-5386-0472-4

Record 187 of 491

Title: Interference of Data Transmission in Access and Backbone Networks by High-Power Sensor System

Author(s): Munster, P (Munster, Petr); Horvath, T (Horvath, Tomas); Vojtech, J (Vojtech, Josef); Havlis, O (Havlis, Ondrej); Slapak, M (Slapak, Martin); Skoda, P (Skoda, Pavel); Radil, J (Radil, Jan); Velc, R (Velc, Radek); Hula, M (Hula, Miloslav)

Source: FIBER AND INTEGRATED OPTICS **Volume:** 36 **Issue:** 3 **Pages:** 144-156 **DOI:** 10.1080/01468030.2017.1327624 **Published:** 2017

Abstract: Currently, individual optical fibers are mostly used for each non-data application, which is very inefficient and uneconomical. Sharing a single fiber for multiple applications is a promising solution. However, in the case of a non-data application, the situation is much more complicated compared to data because of special application ' s requirements. In laboratory setup, we performed a measurement with a standard G.652D optical fiber for analyzing possible interaction of stable frequency/accurate time transmission, 1.25/10Gbps data transmission (typical bitrates for access point-to-point networks), and high-power sensor signal for different channel spacing and different pulse duration of sensor signal.

Accession Number: WOS:000402716400005

ISSN: 0146-8030

eISSN: 1096-4681

Record 188 of 491

Title: Modeling sgB[e] Circumstellar Disks

Author(s): Kurfurst, P (Kurfurst, P.); Feldmeier, A (Feldmeier, A.); Krticka, J (Krticka, J.)

Edited by: Miroshnichenko A; Zharikov S; Korcakova D; Wolf M

Source: B(E) PHENOMENON: FORTY YEARS OF STUDIES **Book Series:** Astronomical Society of the Pacific Conference Series **Volume:** 508 **Pages:** 17-22 **Published:** 2017

Abstract: During their evolution, massive stars are characterized by a significant loss of mass either via spherically symmetric stellar winds or by aspherical mass-loss mechanisms, namely outflowing equatorial disks. However, the scenario that leads to the formation of a disk or rings of gas and dust around these objects is still under debate. Is it a viscous disk or an ouftlowing disk-forming wind or some other mechanism? It is also unclear how various physical mechanisms that act on the circumstellar environment of the stars affect its shape, density, kinematic, and thermal structure. We assume that the disk-forming mechanism is a viscous transport within an equatorial outflowing disk of a rapidly or even critically rotating star. We study the hydrodynamic and thermal structure of optically thick dense parts of outflowing circumstellar disks that may form around,e.g., Be stars, sgB[e] stars, or

Pop m stars. We calculate self-consistent time dependent models of the inner dense region of the disk that is strongly affected either by irradiation from the central star and by contributions of viscous heating effects. We also simulate the dynamic effects of collision between expanding ejecta of supernovae and circumstellar disks that may be form in sgB[e] stars and, e.g., LBVs or Pop in stars.

Accession Number: WOS:000401591600003

Conference Title: Conference on B(e) Phenomenon: Forty Years of Studies

Conference Date: JUN 27-JUL 01, 2016

Conference Location: Charles Univ, Comp Sci Inst, Prague, CZECH REPUBLIC

Conference Sponsors: Universidad Nacl Autonoma Mexico, Univ N Carolina Greensboro, Coll Arts & Sci Advancement Council, Univ N Carolina Greensboro, Dept Phys & Astronomy, Charles Univ Prague, Astron Inst

Conference Host: Charles Univ, Comp Sci Inst

ISBN: 978-1-58381-900-5

Record 189 of 491

Title: Rayleigh Scattering by Helium in Stellar Atmospheres

Author(s): Fisak, J (Fisak, J.); Kubat, J (Kubat, J.); Krticka, J (Krticka, J.)

Edited by: Miroshnichenko A; Zharikov S; Korcakova D; Wolf M

Source: B(E) PHENOMENON: FORTY YEARS OF STUDIES **Book Series:** Astronomical Society of the Pacific Conference Series **Volume:** 508 **Pages:** 115-120 **Published:** 2017

Abstract: We study the influence of Rayleigh scattering by helium on synthetic spectra and stellar atmosphere models. Rayleigh scattering by helium is often neglected in hot star atmosphere models. This approximation is justified by the small population of helium in stars with solar composition (about 10% by number) and lower Rayleigh scattering total cross section of helium with respect to neutral hydrogen. However, for stars with large helium abundances Rayleigh scattering by helium can be a significant opacity source.

Accession Number: WOS:000401591600017

Conference Title: Conference on B(e) Phenomenon: Forty Years of Studies

Conference Date: JUN 27-JUL 01, 2016

Conference Location: Charles Univ, Comp Sci Inst, Prague, CZECH REPUBLIC

Conference Sponsors: Universidad Nacl Autonoma Mexico, Univ N Carolina Greensboro, Coll Arts & Sci Advancement Council, Univ N Carolina Greensboro, Dept Phys & Astronomy, Charles Univ Prague, Astron Inst

Conference Host: Charles Univ, Comp Sci Inst

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kubat, Jiri	G-9032-2014	0000-0003-4269-8278

ISBN: 978-1-58381-900-5

Record 190 of 491

Title: Tensorial elastic properties and stability of interface states associated with Sigma 5(210) grain boundaries in Ni-3(Al,Si)

Author(s): Friak, M (Friak, Martin); Vsianska, M (Vsianska, Monika); Holec, D (Holec, David); Zeleny, M (Zeleny, Martin); Sob, M (Sob, Mojmir)

Source: SCIENCE AND TECHNOLOGY OF ADVANCED MATERIALS **Volume:** 18 **Issue:** 1 **Pages:** 273-282 **DOI:** 10.1080/14686996.2017.1312519 **Published:** 2017

Abstract: Grain boundaries (GBs) represent one of the most important types of defects in solids and their instability leads to catastrophic failures in materials. Grain boundaries are challenging for theoretical studies because of their distorted atomic structure. Fortunately, quantum-mechanical methods can reliably compute their properties. We calculate and analyze (tensorial) anisotropic elastic properties of periodic approximants of interface states associated with GBs in one of the most important intermetallic compounds for industrial applications, Ni3Al, appearing in Ni-based superalloys. Focusing on the Sigma 5(210) GBs as a case study, we assess the mechanical stability of the corresponding interface states by checking rigorous elasticity-based Born stability criteria. The critical elastic constant is found three-/five-fold softer contributing thus to the reduction of the mechanical stability of Ni3Al polycrystals (experiments show their GB-related failure). The tensorial elasto-chemical complexity of interface states associated with the studied GBs exemplifies itself in high sensitivity of elastic constants to the GB composition. As another example we study the impact caused by Si atoms segregating into the atomic layers close to the GB and substituting Al atoms. If wisely exploited, our study paves the way towards solute-controlled design of GB-related interface states with controlled stability and/or tensorial properties. [GRAPHICS]

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Accession Number: WOS:000400382000001

PubMed ID: 28567173

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zeleny, Martin	C-5602-2013	0000-0001-6715-4088

ISSN: 1468-6996

eISSN: 1878-5514

Record 191 of 491

Title: Behavior of sphingomyelin and ceramide in a tear film lipid layer model

Author(s): Olzynska, A (Olzynska, Agnieszka); Cwiklik, L (Cwiklik, Lukasz)

Source: ANNALS OF ANATOMY-ANATOMISCHER ANZEIGER **Volume:** 210 **Pages:** 128-134 **DOI:** 10.1016/j.aanat.2016.10.005 **Published:** 2017

Abstract: Tear film lipid layer is a complex lipid mixture forming the outermost interface between eye and environment. Its key characteristics, such as surface tension and structural stability, are governed by the presence of polar lipids. The origin of these lipids and exact composition of the mixture are still elusive. We focus on two minor polar lipid components of the tear film lipid later: sphingomyelin and ceramide. By employing coarse grain molecular dynamics in silico simulations accompanied by Langmuir balance experiments we provide molecular-level insight into behavior of these two lipids in a tear film lipid layer model. Sphingomyelin headgroups are significantly exposed at the water-lipids boundary while ceramide molecules are incorporated between other lipids frequently interacting with nonpolar lipids. Even though these two lipids increase surface tension of the film, their molecular-level behavior suggests that they have a stabilizing effect on the tear film lipid layer.

Accession Number: WOS:000395610600016

PubMed ID: 27837653

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Olzynska, Agnieszka	F-5152-2014	
Cwiklik, Lukasz	A-7206-2008	0000-0002-2083-8738

ISSN: 0940-9602

eISSN: 1618-0402

Record 192 of 491

Title: Satellite DNA and Transposable Elements in Seabuckthorn (Hippophae rhamnoides), a Dioecious Plant with Small Y and Large X Chromosomes

Author(s): Puterova, J (Puterova, Janka); Razumova, O (Razumova, Olga); Martinek, T (Martinek, Tomas); Alexandrov, O (Alexandrov, Oleg); Divashuk, M (Divashuk, Mikhail); Kubat, Z (Kubat, Zdenek); Hobza, R (Hobza, Roman); Karlov, G (Karlov, Gennady); Kejnovsky, E (Kejnovsky, Eduard)

Source: GENOME BIOLOGY AND EVOLUTION **Volume:** 9 **Issue:** 1 **Pages:** 197-212 **DOI:** 10.1093/gbe/evw303 **Published:** JAN 2017

Abstract: Seabuckthorn (Hippophae rhamnoides) is a dioecious shrub commonly used in the pharmaceutical, cosmetic, and environmental industry as a source of oil, minerals and vitamins. In this study, we analyzed the transposable elements and satellites in its genome. We carried out Illumina DNA sequencing and reconstructed the main repetitive DNA sequences. For data analysis, we developed a new bioinformatics approach for advanced satellite DNA analysis and showed that about 25% of the genome consists of satellite DNA and about 24% is formed of transposable elements, dominated by Ty3/Gypsy and Ty1/Copia LTR retrotransposons. FISH mapping revealed X chromosome-accumulated, Y

chromosome-specific or both sex chromosomes-accumulated satellites but most satellites were found on autosomes. Transposable elements were located mostly in the subtelomeres of all chromosomes. The 5S rDNA and 45S rDNA were localized on one autosomal locus each. Although we demonstrated the small size of the Y chromosome of the seabuckthorn and accumulated satellite DNA there, we were unable to estimate the age and extent of the Y chromosome degeneration. Analysis of dioecious relatives such as Shepherdia would shed more light on the evolution of these sex chromosomes.

Accession Number: WOS:000396057400016

PubMed ID: 28057732

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Karlov, Gennady	F-7403-2013	0000-0002-9016-103X
Razumova, Olga	N-1037-2016	
Hobza, Roman	I-4297-2014	
Kubat, Zdenek	D-9221-2012	0000-0001-8278-9495
Divashuk, Mikhail		0000-0001-6221-3659

ISSN: 1759-6653

Record 193 of 491

Title: Aromaticity, the Huckel 4n+2 Rule and Magnetic Current

Author(s): Zhao, LL (Zhao, Lili); Grande-Aztatzi, R (Grande-Aztatzi, Rafael); Foroutan-Nejad, C (Foroutan-Nejad, Cina); Ugalde, JM (Ugalde, Jesus M.); Frenking, G (Frenking, Gernot)

Source: CHEMISTRYSELECT **Volume:** 2 **Issue:** 3 **Pages:** 863-870 **DOI:** 10.1002/slct.201602080 **Published:** JAN 2017

Abstract: Quantum chemical calculations using density functional theory and correlated ab initio methods of the 10 pi-electron systems (N6H6)(2+) and C2N4H6 show that the planar forms are no minima on the potential energy surfaces. The twisted ring structures of the two species are energy minima, but acyclic isomers are much lower in energy. The planar geometries sustain strong diamagnetic ring current comparable with that of benzene. In contrast, the calculated multicenter normalized Giambiagi electron delocalization index ING suggests that pi- delocalization in planar (N6H6)(2+) and C2N4H6 is much weaker than in benzene. Since aromaticity is synonymous for a particular stability of cyclic delocalized systems, it may be stated that calculation or measurement of magnetic chemical shifts due to induced ring currents is not a reliable method to ascertain the aromatic character of a molecule. Aromatic compounds exhibit ring current induced magnetic shielding, but the reverse conclusion that ring current induced magnetic shielding identifies aromaticity is not justified. Furthermore, the 4n+ 2 rule as indicator of aromatic stabilization should only be used in conjunction with the ring size; the nature of the occupied pi orbitals must always be examined.

Accession Number: WOS:000395533100003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
DONOSTIA INTERNATIONAL PHYSICS CTR., DIPC	C-3171-2014	
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Grande-Aztatzi, Rafael	G-4660-2015	0000-0002-1919-4883

ISSN: 2365-6549

Record 194 of 491

Title: Molecular Dimensions and Porous Structure of Activated Carbons for Sorption of Xylene and Isooctane

Author(s): Troppova, I (Troppova, Ivana); Matejova, L (Matejova, Lenka); Kubonova, L (Kubonova, Lenka); Strasak, T (Strasak, Tomas); Studentova, S (Studentova, Sona); Kustrowski, P (Kustrowski, Piotr); Obalova, L (Obalova, Lucie)

Source: CHEMICAL ENGINEERING & TECHNOLOGY **Volume:** 40 **Issue:** 1 **Pages:** 6-17 **DOI:** 10.1002/ceat.201500675 **Published:** JAN 2017

Abstract: The sorption of xylene and isooctane was measured by the gravimetric flow sorption method on commercial activated carbons (ACs), namely, virgin and reactivated ACs. Nitrogen physisorption, high-pressure mercury porosimetry, helium pycnometry, iodine number, pH measurement, Raman and X-ray photoelectron spectroscopies were applied for textural, structural, and surface characterization of ACs. The equilibrium geometries of isooctane and xylene molecules were modeled using density functional theory (DFT) calculations. Their dimensions were estimated to be correlated with textural properties of ACs to reveal the effect of size selectivity. The key factors influencing the adsorption capacity of the chosen ACs for both tested volatile organic compounds (VOCs) were found to be the mesopore surface area and the surface basicity.

Accession Number: WOS:000393855200001

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Strasak, Tomas	H-3493-2014	0000-0001-6413-0494

ISSN: 0930-7516

eISSN: 1521-4125

Record 195 of 491

Title: Urinary Neutrophil Gelatinase-Associated Lipocalin Does Not Distinguish Acute Rejection from Other Causes of Acute Kidney Injury in Pediatric Renal Transplant Recipients

Author(s): Seeman, T (Seeman, Tomas); Vondrak, K (Vondrak, Karel); Dusek, J (Dusek, Jiri); Simankova, N (Simankova, Nadezda); Zieg, J (Zieg, Jakub); Hacek, J (Hacek, Jaromir); Chadimova, M (Chadimova, Maria); Sopko, B (Sopko, Bruno); Fortova, M (Fortova, Magdalena)

Source: CLINICAL LABORATORY **Volume:** 63 **Issue:** 1 **Pages:** 111-114 **DOI:** 10.7754/Clin.Lab.2016.160702 **Published:** 2017

Abstract: Background: The aim of this prospective single center study was to investigate the ability of urinary neutrophil gelatinase-associated lipocalin (NGAL) to distinguish acute rejection from other causes of acute kidney injury (AM) in children after renal transplantation.

Methods: Fifteen children fulfilled the inclusion criteria (acute kidney injury (AKI) with allograft biopsy, at least 21 days after renal transplantation, no sepsis) during 2013 - 2014 in our pediatric transplantation center. The mean age was 14.8 +/- 2.8, median time after renal transplantation was 0.4 years (range 0.1 - 3.8). Urinary NGAL was measured in spot urine by Chemiluminescent Microparticle Immunoassay technology.

Results: Four patients had biopsy proven acute rejection (rejection group), eleven children had AM of other cause (non-rejection group). The median urinary NGAL concentration in the rejection group was not significantly different from NGAL in the non-rejection group (7.3 ng/mL, range 3.0 - 42.3 vs. 8.6 ng/mL, range 3.4 - 54.7, $p = 0.48$). There was a significant negative correlation between eGFR and urinary NGAL concentrations ($r = -0.77$, $p < 0.001$).

Conclusions: Our small study suggests that in children after renal transplantation, urinary NGAL cannot be used as a specific marker for distinguishing acute rejection from other non-rejection causes of AM. Urinary NGAL was mainly associated with graft function but not with the etiology of AKI.

Accession Number: WOS:000392043100015

PubMed ID: 28164508

ISSN: 1433-6510

Record 196 of 491

Title: Improvement of the visibility of concealed features in artwork NIR reflectograms by information separation

Author(s): Blazek, J (Blazek, Jan); Striova, J (Striova, Jana); Fontana, R (Fontana, Raffaella); Zitova, B (Zitova, Barbara)

Source: DIGITAL SIGNAL PROCESSING **Volume:** 60 **Pages:** 140-151 **DOI:** 10.1016/j.dsp.2016.09.007 **Published:** JAN 2017

Abstract: Near Infrared (NIR) reflectography, coupled to visible (VIS) one, is a spectrophotometric imaging technique employed to probe both the inner and the outer layers of artworks. NIR reflectograms may partially contain information pertinent to the visible spectrum (due to the poor pigment transparency in NIR) and this decreases their comprehensibility. This work presents an innovative digital processing methodology for accentuating information contained in the infrared reflectograms. The proposed method consists of inducing minor changes in pixel intensity by suppressing VIS information content from NIR information content. The method creates such enhanced NIR reflectogram by extrapolating VIS reflectogram to a reflectogram recorded in NIR range and by subtracting it from the measured values in the near infrared spectral sub-band. As an extrapolator we suggest a feed forward artificial neural network (ANN). Significant results of improved visualization are exemplified on reflectograms acquired with a VIS-NIR (400, 2250) nm scanning device on real paintings such as Madonna dei Fusi attributed to Leonardo da Vinci. Parameters of the method, artificial neural network and separability of used pigments are discussed.

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ISSN: 1051-2004
eISSN: 1095-4333

Record 197 of 491

Title: Scaffold analysis of PubChem database as background for hierarchical scaffold-based visualization

Author(s): Velkoborsky, J (Velkoborsky, Jakub); Hoksza, D (Hoksza, David)

Source: JOURNAL OF CHEMINFORMATICS **Volume:** 8 **Article Number:** 74 **DOI:** 10.1186/s13321-016-0186-7 **Published:** DEC 29 2016

Abstract: Background: Visualization of large molecular datasets is a challenging yet important topic utilised in diverse fields of chemistry ranging from material engineering to drug design. Especially in drug design, modern methods of high-throughput screening generate large amounts of molecular data that call for methods enabling their analysis. One such method is classification of compounds based on their molecular scaffolds, a concept widely used by medicinal chemists to group molecules of similar properties. This classification can then be utilized for intuitive visualization of compounds.
Results: In this paper, we propose a scaffold hierarchy as a result of large-scale analysis of the PubChem Compound database. The analysis not only provided insights into scaffold diversity of the PubChem Compound database, but also enables scaffold-based hierarchical visualization of user compound data sets on the background of empirical chemical space, as defined by the PubChem data, or on the background of any other user-defined data set. The visualization is performed by a web based client-server application called Scaffvis. It provides an interactive zoomable tree map visualization of data sets up to hundreds of thousands molecules. Scaffvis is free to use and its source codes have been published under an open source license.

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PubMed ID: 28090217

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Hoksza, David		0000-0003-4679-0557

ISSN: 1758-2946

Record 198 of 491

Title: Thermodynamics of supersaturated steam: Molecular simulation results

Author(s): Moucka, F (Moucka, Filip); Nezbeda, I (Nezbeda, Ivo)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 145 **Issue:** 24 **Article Number:** 244501 **DOI:** 10.1063/1.4972411 **Published:** DEC 28 2016

Abstract: Supersaturated steam modeled by the Gaussian charge polarizable model [P. Paricaud, M. Predota, and A. A. Chialvo, J. Chem. Phys. 122, 244511 (2005)] and BK3 model [P. Kiss and A. Baranyai, J. Chem. Phys. 138, 204507 (2013)] has been simulated at conditions occurring in steam turbines using the multiple-particle-move Monte Carlo for both the homogeneous phase and also implemented for the Gibbs ensemble Monte Carlo molecular simulation methods. Because of these thermodynamic conditions, a specific simulation algorithm has been developed to bypass common simulation problems resulting from very low densities of steam and cluster formation therein. In addition to pressure-temperature-density and orthobaric data, the distribution of clusters has also been evaluated. The obtained extensive data of high precision should serve as a basis for development of reliable molecular-based equations for properties of metastable steam. Published by AIP Publishing.

Accession Number: WOS:000392174800035
PubMed ID: 28049313
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Record 199 of 491

Title: Theoretical investigation of the structural, electronic, magnetic and elastic properties of binary cubic C15-Laves phases TbX2 (X = Co and Fe)

Author(s): Bentouaf, A (Bentouaf, A.); Mebsout, R (Mebsout, R.); Rached, H (Rached, H.); Amari, S (Amari, S.); Reshak, AH (Reshak, A. H.); Aissa, B (Aissa, B.)

Source: JOURNAL OF ALLOYS AND COMPOUNDS **Volume:** 689 **Pages:** 885-893 **DOI:** 10.1016/j.jallcom.2016.08.046 **Published:** DEC 25 2016

Abstract: We report on a comprehensive theoretical investigation of the physical properties of the cubic MgCu2-type binary Laves phases TbCo2 and TbFe2 compounds. The density functional full-potential linearized augmented planewave (FP-LAPW) method was used. We adopted the generalized gradient approximation (GGA) to estimate the exchange correlation potential and the GGA+U (i.e. Hubbard correction) calculations in accurately characterizing the correlation effects. The lattice parameter a(0), bulk modulus B and magnetic moment M at the equilibrium state were found to well corroborate the experimental data. We have calculated the magnetic moments of Co and Fe in the TbCo2 and TbFe2, respectively, by using GGA and GGA+U methods, where the magnetic moments value of Fe was found to be higher than that of Co. The GGA+U gave higher value than that obtained by GGA. To obtain further insight into the type of states associated with each orbital, the projected density of states of the Co-3d and Fe-3d orbitals were calculated using GGA and GGA+U, respectively. This work highlights the role of the correlated electrons processing for an accurate description of these binary Laves phases compounds. (C) 2016 Published by Elsevier B.V.

Accession Number: WOS:000384427200114

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363
RACHED, Habib		0000-0003-3867-576X

ISSN: 0925-8388
eISSN: 1873-4669

Record 200 of 491

Title: Optical spectroscopy and system-bath interactions in molecular aggregates with full configuration interaction Frenkel exciton model

Author(s): Seibt, J (Seibt, Joachim); Slama, V (Slama, Vladislav); Mancal, T (Mancal, Tomas)

Source: CHEMICAL PHYSICS **Volume:** 481 **Pages:** 218-230 **DOI:** 10.1016/j.chemphys.2016.08.017 **Published:** DEC 20 2016

Abstract: Standard application of the Frenkel exciton model neglects resonance coupling between collective molecular aggregate states with different number of excitations. These inter-band coupling terms are, however, of the same magnitude as the intra-band coupling between singly excited states. We systematically derive the Frenkel exciton model from quantum chemical considerations, and identify it as a variant of the configuration interaction method. We discuss all non-negligible couplings between collective aggregate states, and provide compact formulae for their calculation. We calculate absorption spectra of molecular aggregate of carotenoids and identify significant band shifts as a result of inter-band coupling. The presence of inter-band coupling terms requires renormalization of the system-bath coupling with respect to standard formulation, but renormalization effects are found to be weak. We present detailed discussion of molecular dimer and calculate its time-resolved two-dimensional Fourier transformed spectra to find weak but noticeable effects of peak amplitude redistribution due to inter-band coupling. (C) 2016 Published by Elsevier B.V.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Slama, Vladislav	Q-3330-2017	0000-0001-7339-5523

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Page 5 (Records 201 -- 250)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 201 of 491

Title: Spatial distribution and risk assessment of metals in agricultural soils

Author(s): Bednarova, Z (Bednarova, Zdenka); Kalina, J (Kalina, Jiri); Hajek, O (Hajek, Ondrej); Sanka, M (Sanka, Milan); Komprdova, K (Komprdova, Klara)

Source: GEODERMA **Volume:** 284 **Pages:** 113-121 **DOI:** 10.1016/j.geoderma.2016.08.021 **Published:** DEC 15 2016

Abstract: The purpose of the presented study was to identify possible ecological and health risks by metal contamination in soil. More than 50,000 topsoil samples in agricultural soil were used to evaluate spatial concentrations and risks posed by selected metals on a national scale. Variograms and correlograms were used to identify metal spatial patterns and appropriate sampling distances. All metals were spatially dependent on short distances (up to 7 km). Optimal sampling densities to detect contamination at the local scale were estimated to be at around 1 sample per 0.5 km for Cd, Cu and Zn and 1.5-2 km for Pb, Hg and Ni based on Moran's index = 0.7. The concentrations of metals were partly influenced by precipitation and pH, but mostly by geology and industry. The Kriging method was used to create interpolated maps for individual metals. High concentrations of Cd, Pb and Zn were found in well-known mining areas (the Ore Mountains, the Upper Silesian Basin, the towns of Kutna Hora and Vibram). Elevated Ni and Hg concentrations resulted mainly from the nature of the parent rock material. Cu contamination was specifically influenced by Cu-based fungicides applied on soils where hop and wine are grown. Czech and European legal limits for various pH and soil textures were applied to identify potential risk areas. A relatively large area of agricultural soil (16%) is above the prevention limit for at least one metal. However, only a few localities exceed the limits with respect to food chain contamination and the inhibition of plant growth. Comparison of our results with European studies (LUCAS, GEMAS, FOREGS) points to the need for high density sampling in order to conduct accurate risk assessment and demonstrates that serious soil contamination happens (and needs monitoring) at the local and not the continental scale. (C) 2016 Elsevier B.V. All rights reserved.

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Record 202 of 491

Title: Evaluation of gas-particle partitioning in a regional air quality model for organic pollutants

Author(s): Efstathiou, CI (Efstathiou, Christos I.); Matejovicova, J (Matejovicova, Jana); Bieser, J (Bieser, Johannes); Lammel, G (Lammel, Gerhard)

Source: ATMOSPHERIC CHEMISTRY AND PHYSICS **Volume:** 16 **Issue:** 23 **Pages:** 15327-15345 **DOI:** 10.5194/acp-16-15327-2016 **Published:** DEC 9 2016

Abstract: Persistent organic pollutants (POPs) are of considerable concern due to their well-recognized toxicity and their potential to bioaccumulate and engage in long-range transport. These compounds are semi-volatile and, therefore, create a partition between vapour and condensed phases in the atmosphere, while both phases can undergo chemical reactions. This work describes the extension of the Community Multiscale Air Quality (CMAQ) modelling system to POPs with a focus on establishing an adaptable framework that accounts for gaseous chemistry, heterogeneous reactions, and gas-particle partitioning (GPP). The effect of GPP is assessed by implementing a set of independent parameterizations within the CMAQ aerosol module, including the Junge-Pankow (JP) adsorption model, the Harner-Bidleman (HB) organic matter (OM) absorption model, and the dual Dachs-Eisenreich (DE) black carbon (BC) adsorption and OM absorption model. Use of these descriptors in a modified version of CMAQ for benzo[a]pyrene (BaP) results in different fate and transport patterns as demonstrated by regional-scale simulations performed for a European domain during 2006. The dual DE model predicted 24.1% higher average domain concentrations compared to the HB model, which was in turn predicting 119.2% higher levels compared to the baseline JP model. Evaluation with measurements from the European Monitoring and Evaluation Programme (EMEP) reveals the capability of the more extensive DE model to better capture the ambient levels and seasonal behaviour of BaP. It is found that the heterogeneous reaction of BaP with O-3 may decrease its atmospheric lifetime by 25.2% (domain and annual average) and near-ground concentrations by 18.8 %. Marginally better model performance was found for one of the six EMEP stations (Kosetice) when heterogeneous BaP reactivity was included. Further analysis shows that, for the rest of the EMEP locations, the model continues to underestimate BaP levels, an observation that can be attributed to low emission estimates for such remote areas. These findings suggest that, when modelling the fate and transport of organic pollutants on large spatio-temporal scales, the selection and parameterization of GPP can be as important as degradation (reactivity).

Accession Number: WOS:000390767800005

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bieser, Johannes	R-2583-2017	0000-0003-2938-3124
Lammel, Gerhard		0000-0003-2313-0628

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Record 203 of 491

Title: Structural changes in the Czech, Slovak and euro area economies during the Great Recession

Author(s): Tvrz, S (Tvrz, Stanislav); Vasicek, O (Vasicek, Osvald)

Source: REVIEW OF ECONOMIC PERSPECTIVES **Volume:** 16 **Issue:** 4 **Pages:** 297-336 **DOI:** 10.1515/revecp-2016-0018 **Published:** DEC 2016

Abstract: The goal of this paper is to identify and compare the most important changes in the structure of the Czech economy, as a small open economy with independent monetary policy, the Slovak economy, as a small open economy that entered monetary union, and the economy of the euro area, which has a common monetary policy, during the turbulent period of the Great Recession, the subsequent anaemic recovery and recent disinflationary period. Structural changes are identified with the help of nonlinear dynamic stochastic models of general equilibrium with time-varying parameters. The model parameters are estimated using Bayesian methods and a nonlinear particle filter. The results confirm the similarity of the Czech and Slovak economies and show that in certain respects the structure of the Czech economy might be closer to that of the euro area than that of Slovakia. The time-varying estimates reveal many similarities between the parameter changes in the Czech economy and those in the euro area. In Slovakia, the situation during the Great Recession was dominated by the country's adoption of the euro, which caused large deviations in its Calvo parameters.

Accession Number: WOS:000406945200002

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eISSN: 1804-1663

Record 204 of 491

Title: Absence of positive selection on CenH3 in Luzula suggests that holokinetic chromosomes may suppress centromere drive

Author(s): Zedek, F (Zedek, Frantisek); Bures, P (Bures, Petr)

Source: ANNALS OF BOTANY **Volume:** 118 **Issue:** 7 **Pages:** 1347-1352 **DOI:** 10.1093/aob/mcw186 **Published:** DEC 2016

Abstract: Background and Aims The centromere drive theory explains diversity of eukaryotic centromeres as a consequence of the recurrent conflict between centromeric repeats and centromeric histone H3 (CenH3), in which selfish centromeres exploit meiotic asymmetry and CenH3 evolves adaptively to counterbalance deleterious consequences of driving centromeres. Accordingly, adaptively evolving CenH3 has so far been observed only in eukaryotes with asymmetric meiosis. However, if such evolution is a consequence of centromere drive, it should depend not only on meiotic asymmetry but also on monocentric or holokinetic chromosomal structure. Selective pressures acting on CenH3 have never been investigated in organisms with holokinetic meiosis despite the fact that holokinetic chromosomes have been hypothesized to suppress centromere drive. Therefore, the present study evaluates selective pressures acting on the CenH3 gene in holokinetic organisms for the first time, specifically in the representatives of the plant genus Luzula (Juncaceae), in which the kinetochore formation is not co-localized with any type of centromeric repeat.
Methods PCR, cloning and sequencing, and database searches were used to obtain coding CenH3 sequences from Luzula species. Codon substitution models were employed to infer selective regimes acting on CenH3 in Luzula.
Key Results In addition to the two previously published CenH3 sequences from L. nivea, 16 new CenH3 sequences have been isolated from 12 Luzula species. Two CenH3 isoforms in Luzula that originated by a duplication event prior to the divergence of analysed species were found. No signs of positive selection acting on CenH3 in Luzula were detected. Instead, evidence was found that selection on CenH3 of Luzula might have been relaxed.
Conclusions The results indicate that holokinetism itself may suppress centromere drive and, therefore, holokinetic chromosomes might have evolved as a defence against centromere drive.

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PubMed ID: 27616209

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zedek, Frantisek		0000-0003-1593-1775

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eISSN: 1095-8290

Record 205 of 491

Title: Ion Pathways in the Na+/K+-ATPase

Author(s): Cechova, P (Cechova, Petra); Berka, K (Berka, Karel); Kubala, M (Kubala, Martin)

Source: JOURNAL OF CHEMICAL INFORMATION AND MODELING **Volume:** 56 **Issue:** 12 **Pages:** 2434-2444 **DOI:** 10.1021/acs.jcim.6b00353 **Published:** DEC 2016

Abstract: Na+/K+-ATPase (NKA) is an essential cation pump protein responsible for the maintenance of the sodium and potassium gradients across the plasma membrane. Recently published high-resolution structures revealed amino acids forming the cation binding sites (CBS) in the transmembrane domain and variable position of the domains in the cytoplasmic headpiece. Here we report molecular dynamic simulations of the human NKA alpha 1 beta 1 isoform embedded into DOPC bilayer. We have analyzed the NKA conformational changes in the presence of Na+- or K+-cations in the CBS, for various combinations of the cytoplasmic ligands, and the two major enzyme conformations in the 100 ns runs (more than 2.5 mu s of simulations in total). We identified two novel cytoplasmic pathways along the pairs of transmembrane helices TM3/TM7 or TM6/TM9 that allow hydration of the CBS or transport of cations from/to the bulk. These findings can provide a structural explanation for previous mutagenesis studies, where mutation of residues that are distal from the CBS resulted in the alteration of the enzyme affinity to the transported cations or change in the enzyme activity.

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PubMed ID: 27966362

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Berka, Karel	E-2839-2010	0000-0001-9472-2589
Cechova, Petra		0000-0002-5069-6398

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Record 206 of 491

Title: Different QM/MM Approaches To Elucidate Enzymatic Reactions: Case Study on ppGalNAcT2

Author(s): Janos, P (Janos, Pavel); Trnka, T (Trnka, Tomas); Kozmon, S (Kozmon, Stanislav); Tvaroska, I (Tvaroska, Igor); Koca, J (Koca, Jaroslav)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 12 **Issue:** 12 **Pages:** 6062-6076 **DOI:** 10.1021/acs.jctc.6b00531 **Published:** DEC 2016

Abstract: Hybrid QM/MM computational studies can provide invaluable insight into the mechanisms of enzymatic reactions that can be exploited for rational drug design. Various approaches are available for such studies. However, their strengths and weaknesses may not be immediately apparent. Using the retaining glycosyltransferase ppGalNAcT2 as a case study, we compare different methodologies used to obtain reaction paths and transition state information. Ab Initio MD using CPMD coupled with the String Method is used to derive the minimum free energy reaction path. The geometrical features of the free energy path, especially around the transition state, agree with the minimum potential energy path obtained by the much less computationally expensive Nudged Elastic Band method. The barrier energy, however, differs by 8 kcal/mol. The free energy surface generated by metadynamics provides a rough overview of the reaction and can confirm the physical relevance of optimized paths or provide an initial guess for path optimization methods. Calculations of enzymatic reactions are usually performed at best at the DFT level of theory. A comparison of widely used functionals with high-level DLPNO-CCSD(T)/CBS data on the potential energy profile serves as a validation of the usability of DFT for this type of enzymatic reaction. The M06-2X meta-hybrid functional in particular matches the DLPNO-CCSD(T)/CBS reference extremely well with errors within 1 kcal/mol. However, even pure-GGA functional OPBE provides sufficient accuracy for this type of study.

Accession Number: WOS:000389866500033
PubMed ID: 27787999

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Trnka, Tomas		0000-0002-9273-3820

ISSN: 1549-9618
eISSN: 1549-9626

Record 207 of 491

Title: Microscopic multiphonon method for odd nuclei and its application to O-17

Author(s): De Gregorio, G (De Gregorio, G.); Knapp, F (Knapp, F.); Lo Iudice, N (Lo Iudice, N.); Vesely, P (Vesely, P.)

Source: PHYSICAL REVIEW C **Volume:** 94 **Issue:** 6 **Article Number:** 061301 **DOI:** 10.1103/PhysRevC.94.061301 **Published:** DEC 1 2016

Abstract: An equations of motion phonon method is extended to odd nuclei. It generates an orthonormal basis out of an odd particle coupled to n-phonon core states (n = 0,1,2,...), built of Tamm-Dancoff phonons, and formulates the eigenvalue problem in such a multiphonon particle-core space. O-17 is chosen as testing ground. An intrinsic chiral Hamiltonian is adopted in a large configuration space to perform a calculation using a Hartree-Fock (HF) basis in a space encompassing up to two and, under simplifying assumptions, three phonons. The impact of the different phonon components on spectrum, moments, transitions, and dipole cross section is discussed.

Accession Number: WOS:000389026000001

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290
De Gregorio, Giovanni		0000-0003-0253-915X

ISSN: 2469-9985
eISSN: 2469-9993

Record 208 of 491

Title: Ab initio study of deformed As, Sb, and Bi with an application to thin films

Author(s): Zouhar, M (Zouhar, M.); Sob, M (Sob, M.)

Source: PHYSICAL REVIEW B **Volume:** 94 **Issue:** 18 **Article Number:** 184110 **DOI:** 10.1103/PhysRevB.94.184110 **Published:** NOV 28 2016

Abstract: We present a comprehensive density-functional theory study of total energy and structural properties of As, Sb, and Bi in their A7 ground-state structure and in the bcc, fcc, and simple cubic (sc) modifications. We also investigate continuous structural transitions between these structures. The electronic structures and total energies are calculated both within the generalized gradient approximation (GGA) and local-density approximation (LDA) to the exchange-correlation energy as well as with and without inclusion of the spin-orbit coupling (SOC). The total energies of deformed structures are displayed in contour plots as functions of selected structural parameters and/or atomic volume; these plots are then used for understanding and interpreting structural parameters of As, Sb and Bi thin films on various substrates. Our calculated values of lattice parameters for (0001) thin films of Bi on Si(111) and Ge(111) substrates agree very well with available experimental data. In analogy with that, we suggest to investigate (0001) thin films of As on Ti(0001), Co(0001), Zn(0001) and Rh(111) substrates, of Sb on C(0001), Zn(0001), Al(111), Ag(111) and Au(111) substrates and of Bi on Co(0001), Al(111), Rh(111), Ba(111) and Pb(111) substrates. For these cases, we also predict the lattice parameters of the films. A large part of our results are theoretical predictions which may motivate experimentalists for a deeper study of these systems.

Accession Number: WOS:000388816200003
ISSN: 2469-9950
eISSN: 2469-9969

Record 209 of 491

Title: The impact of nitrogen content and vacancies on structure and mechanical properties of Mo-N thin films

Author(s): Klimashin, FF (Klimashin, F. F.); Koutna, N (Koutna, N.); Euchner, H (Euchner, H.); Holec, D (Holec, D.); Mayrhofer, PH (Mayrhofer, P. H.)

Source: JOURNAL OF APPLIED PHYSICS **Volume:** 120 **Issue:** 18 **Article Number:** 185301 **DOI:** 10.1063/1.4966664 **Published:** NOV 14 2016

Abstract: Based on a combined computational and experimental study, we show that besides the thermodynamically stable beta-MoN0.5 and delta(2)-MoN phases, also metastable gamma-MoNx and its ordered relative gamma'-MoNx can be synthesized by physical vapor deposition. The formation of the NaCl-based gamma-MoNx phase is favored for nitrogen concentrations between 23 and 34 at.% (i.e., x = 0.30-0.53). Higher nitrogen contents (close to the 3:2 stoichiometry, hence, MoN0.67) favor the ordering of the vacancies at the nitrogen sublattice (hence, gamma'-MoNx). The highest hardness of similar to 33 GPa is obtained for single-phase cubic-structured gamma-MoN0.53 coatings, whereas the ordered gamma'-MoN0.67 coatings are slightly softer with a hardness of similar to 28 GPa. (C) 2016 Author(s).

Accession Number: WOS:000388734700023

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mayrhofer, Paul	A-9640-2011	0000-0001-7328-9333
Euchner, Holger		0000-0003-2287-6970
Koutna, Nikola		0000-0001-7901-4736
Klimashin, Fedor F.		0000-0002-2152-7165

ISSN: 0021-8979
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Record 210 of 491

Title: High density ultrashort relativistic positron beam generation by laser-plasma interaction

Author(s): Gu, YJ (Gu, Y. J.); Klimo, O (Klimo, O.); Weber, S (Weber, S.); Korn, G (Korn, G.)

Source: NEW JOURNAL OF PHYSICS **Volume:** 18 **Article Number:** 113023 **DOI:** 10.1088/1367-2630/18/11/113023 **Published:** NOV 9 2016

Abstract: A mechanism of high energy and high density positron beam creation is proposed in ultra-relativistic laser-plasma interaction. Longitudinal electron self-injection into a strong laser field occurs in order to maintain the balance between the ponderomotive potential and the electrostatic potential. The injected electrons are trapped and form a regular layer structure. The radiation reaction and photon emission provide an additional force to confine the electrons in the laser pulse. The threshold density to initiate the longitudinal electron self-injection is obtained from analytical model and agrees with the kinetic simulations. The injected electrons generate gamma-photons which counter-propagate into the laser pulse. Via the Breit-Wheeler process, well collimated positron bunches in the GeV range are generated of the order of the critical plasma density and the total charge is about nano-Coulomb. The above mechanisms are demonstrated by particle-in-cell simulations and single electron dynamics.

Accession Number: WOS:000388515200006

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Gu, Yanjun	G-5767-2014	0000-0002-6234-8489
Klimo, Ondrej	B-2196-2010	0000-0002-0565-2409

ISSN: 1367-2630

Record 211 of 491

Title: Orthology Guided Transcriptome Assembly of Italian Ryegrass and Meadow Fescue for Single-Ncleotide Polymorphism Discovery

Author(s): Stoces, S (Stoces, Stepan); Ruttink, T (Ruttink, Tom); Bartos, J (Bartos, Jan); Studer, B (Studer, Bruno); Yates, S (Yates, Steven); Zwierzykowski, Z (Zwierzykowski, Zbigniew); Abrouk, M (Abrouk, Michael); Roldan-Ruiz, I (Roldan-Ruiz, Isabel); Ksiazczyk, T (Ksiazczyk, Tomasz); Rey, E (Rey, Elodie); Dolezel, J (Dolezel, Jaroslav); Kopecky, D (Kopecky, David)

Source: PLANT GENOME **Volume:** 9 **Issue:** 3 **DOI:** 10.3835/plantgenome2016.02.0017 **Published:** NOV 2016

Abstract: Single-nucleotide polymorphisms (SNPs) represent natural DNA sequence variation. They can be used for various applications including the construction of high-density genetic maps, analysis of genetic variability, genome-wide association studies, and map-based cloning. Here we report on transcriptome sequencing in the two forage grasses, meadow fescue (Festuca pratensis Huds.) and Italian ryegrass (Lolium multiflorum Lam.), and identification of various classes of SNPs. Using the Orthology Guided Assembly (OGA) strategy, we assembled and annotated a total of 18,952 and 19,036 transcripts for Italian ryegrass and meadow fescue, respectively. In addition, we used transcriptome sequence data of perennial ryegrass (L. perenne L.) from a previous study to identify 16,613 transcripts shared across all three species. Large numbers of intraspecific SNPs were identified in all three species: 248,000 in meadow fescue, 715,000 in Italian ryegrass, and 529,000 in perennial ryegrass. Moreover, we identified almost 25,000 interspecific SNPs located in 5343 genes that can distinguish meadow fescue from Italian ryegrass and 15,000 SNPs located in 3976 genes that discriminate meadow fescue from both Lolium species. All identified SNPs were positioned in silico on the seven linkage groups (LGs) of L. perenne using the GenomeZipper approach. With the identification and positioning of interspecific SNPs, our study provides a valuable resource for the grass research and breeding community and will enable detailed characterization of genomic composition and gene expression analysis in prospective Festuca. Lolium hybrids.

Accession Number: WOS:000393120000011
PubMed ID: 27902806

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dolezel, Jaroslav	B-7716-2008	0000-0002-6263-0492
Abrouk, Michael	F-8516-2014	0000-0001-9082-1432
Studer, Bruno	O-2237-2017	
Abrouk, Michael	W-1972-2017	0000-0001-9082-1432
Bartos, Jan	F-6071-2014	

ISSN: 1940-3372

Record 212 of 491

Title: The evolutionary pathway of the staphylococcal cassette chromosome element

Author(s): Indrakova, A (Indrakova, Adela); Maslanova, I (Maslanova, Ivana); Kovacova, V (Kovacova, Viera); Doskar, J (Doskar, Jiri); Pantucek, R (Pantucek, Roman)

Source: BIOLOGIA **Volume:** 71 **Issue:** 11 **Pages:** 1195-1203 **DOI:** 10.1515/biolog-2016-0156 **Published:** NOV 2016

Abstract: The staphylococcal cassette chromosome (SCC) element can carry resistance genes to antibiotics, disinfectants, and heavy metals, contributing to the survival of strains in the environment and causing difficulties in the treatment of staphylococcal infections. Methicillin resistance in staphylococci, which is of particular clinical significance, is encoded by staphylococcal cassette chromosome mec (SCCmec). Despite the importance of the SCC element and description of multiple nucleotide sequences, the information about its origin and evolution is still scarce. Here, we present a phylogenetic analysis of SCC elements that is unique in the use of whole SCC sequences. A phylogenetic tree for a noteworthy number of 81 SCC elements based on global sequence alignment was constructed. The SCC clustering did not reflect the genetic relationships of bacteria containing the SCC elements, but was done according to type, determined by the combination of mec gene complex class and ccr gene complex type. The results emphasise the horizontal gene transfer as a means of spread of SCC elements in bacterial strains. Overall, this study contributes to the understanding of SCC emergence, evolution, and dissemination.

Accession Number: WOS:000391882600001

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Maslanova, Ivana	A-3081-2014	0000-0002-2597-2848
Doskar, Jiri	O-1038-2017	
Pantucek, Roman	P-6758-2014	0000-0002-3950-675X

ISSN: 0006-3088
eISSN: 1336-9563

Record 213 of 491

Title: Lanthanum trilactate: Vibrational spectroscopic study - infrared/Raman spectroscopy

Author(s): Svecova, M (Svecova, Marie); Novak, V (Novak, Vit); Bartunek, V (Bartunek, Vilem); Clupek, M (Clupek, Martin)

Source: VIBRATIONAL SPECTROSCOPY **Volume:** 87 **Pages:** 123-128 **DOI:** 10.1016/j.vibspec.2016.09.020 **Published:** NOV 2016

Abstract: In this study lanthanum trilactate was prepared by neutralization reaction of lactic acid and lanthanum oxide, purified and identified by X-ray powder diffraction. Infrared spectra (Mid-IR region 4000-650 cm(-1)) and Raman spectra (Stokes region 4000-100 cm(-1)) of the high quality crystalline samples have been recorded and presented for the first time. For comparison DFT calculations were performed using Gaussian 09 D.01 and agreement between predicted and measured spectral data has been achieved. Acquired information can be utilized for substance identification for example in various industrial applications or in biological systems. (C) 2016 Elsevier B.V. All rights reserved.
Accession Number: WOS:000389167800018
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Clupek, Martin	A-5823-2009	0000-0003-2773-412X

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Record 214 of 491

Title: Complete genome characterisation and phylogenetic position of Tigray hantavirus from the Ethiopian white-footed mouse, Stenocephalemys albipes
Author(s): de Bellocq, JG (de Bellocq, Joelle Gouey); Tesikova, J (Tesikova, Jana); Meheretu, Y (Meheretu, Yonas); Cizkova, D (Cizkova, Dagmar); Bryjova, A (Bryjova, Anna); Leirs, H (Leirs, Herwig); Bryja, J (Bryja, Josef)
Source: INFECTION GENETICS AND EVOLUTION **Volume:** 45 **Pages:** 242-245 **DOI:** 10.1016/j.meegid.2016.09.009 **Published:** NOV 2016
Abstract: Hantaviruses, well-known human pathogens, have only recently been identified on the African continent. Tigray virus (TIGV) was found in Ethiopia in 2012 in a Murinae species, Stenocephalemys albipes, but the genetic data obtained at that time were too limited to correctly assess its phylogenetic position within the hantavirus tree. We used high throughput sequencing to determine the complete genome of TIGV, which showed a typical hantavirus organisation. The large (L), medium (M), and small (S) genome segments were found to be 6532, 3594 and 1908 nucleotides long, respectively, and the 5' and 3' termini for all three segments were predicted to form the panhandle-like structure typical for bunyaviruses. Nucleotide-based phylogenetic analyses revealed that all three coding segments cluster in the phylogroup III sensu Guo et al. (2013). However, while TIGV S segment is basal to the Murinae-associated hantaviruses, the M and L segments are basal to the Soricomorpha-associated hantaviruses. TIGV is the first Murinae-borne hantavirus showing this inconsistent segmental clustering in the hantavirus phylogenetic tree. We finally propose non-exclusive scenarios that could explain the original phylogenetic position of TIGV. (C) 2016 Elsevier B.V. All rights reserved.
Accession Number: WOS:000388574400032
PubMed ID: 27619058
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bryja, Josef	C-3013-2008	
Meheretu, Yonas	A-2815-2015	
Gouy de Bellocq, Joelle	J-4733-2013	0000-0001-5831-6284

ISSN: 1567-1348
eISSN: 1567-7257

Record 215 of 491

Title: Indenyl Compounds with Constrained Hapticity: The Effect of Strong Intramolecular Coordination
Author(s): Mrozek, O (Mrozek, Ondrej); Vinklarek, J (Vinklarek, Jaromir); Ruzickova, Z (Ruzickova, Zdenka); Honzicek, J (Honzicek, Jan)
Source: EUROPEAN JOURNAL OF INORGANIC CHEMISTRY **Issue:** 33 **Pages:** 5250-5264 **DOI:** 10.1002/ejic.201601029 **Published:** NOV 2016
Abstract: A series of cyclopentadienyl and indenyl molybdenum(II) compounds with intramolecularly coordinated pyridine arms, including scorpionate-like species bearing two irreversibly coordinated arms on the indenyl core, were synthesized and characterized. All presented structural types were confirmed by X-ray diffraction analysis. Owing to the strong nucleophilicity of pyridine, the intramolecular interaction was found to be considerably stronger than that in analogous species bearing tertiary amines in the side chain. Although the starting compounds for the syntheses were isostructural, the reaction outcomes differed considerably. The cyclopentadienyl precursor gave a pentacoordinate (5):N-compound, whereas the indenyl analogue produced a hexacoordinate species with the unprecedented (3):N-coordination mode of the indenyl ligand and thus represents an unusual example of the so-called indenyl effect. The unusually high stability of the (3):N-coordination compounds toward (3) to (5) haptotropic rearrangement was clarified by theoretical calculations. As the strong intramolecular interaction prevented rotation of the indenyl moiety, it could not reach the conformation suitable for the (3) to (5) rearrangement. As a result, the low hapticity was effectively locked.
Accession Number: WOS:000388494000010
ISSN: 1434-1948
eISSN: 1099-0682

Record 216 of 491

Title: Synthesis and catalytic activity of ruthenium complexes modified with chiral racemic per- and polyfluorooxaalkanoates
Author(s): Lipovska, P (Lipovska, Pavlina); Rathouska, L (Rathouska, Lucie); Simunek, O (Simunek, Onrej); Hosek, J (Hosek, Jan); Kolarikova, V (Kolarikova, Viola); Rybackova, M (Rybackova, Marketa); Cvacka, J (Cvacka, Josef); Svoboda, M (Svoboda, Martin); Kvicala, J (Kvicala, Jaroslav)
Source: JOURNAL OF FLUORINE CHEMISTRY **Volume:** 191 **Pages:** 14-22 **DOI:** 10.1016/j.jfluchem.2016.09.005 **Published:** NOV 2016
Abstract: Silver salts of racemic 2H-perfluoro(3-oxahexanoic) (3a), perfluoro(2-methyl-3-oxahexanoic) (3b) and 2,3,3,3-tetrafluoro-2-methoxypropanoic acid (3c) gave with Hoveyda-Grubbs 2nd generation catalyst 4 or its bis(polyfiuoroalkylated) analogue 5 the corresponding bis(polyfluoroacylated) ruthenium complexes 1a-1c or 2a, 2b as mixtures of three diastereoisomers. Their catalytic activity in model ring-closing metathesis (RCM) reactions decreased in the order 1b-2b > 1a-2a > 1c due to increased steric hindrance around the catalytic centre in complexes 1a, 1c and 2a, as well as due to lower acidity of acid 3c resulting in lower electrophilicity of the complex 1c. Thus, the complexes 1b and 2b displayed high activity in RCM of bis-unsaturated malonates forming disubstituted (RCM2) or trisubstituted (RCM3) double bond and were even significantly active in the formation of tetrasubstituted bond (RCM4), while complexes 1a, 1c were active in RCM2 but inactive in RCM3. Moreover, the yield of RCM2 catalyzed with complex is was rather low. (C) 2016 Elsevier B.V. All rights reserved.
Accession Number: WOS:000388058300002
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cvacka, Josef		0000-0002-3590-9009
Kvicala, Jaroslav		0000-0002-9713-021X

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Record 217 of 491

Title: Variation of 45S rDNA intergenic spacers in Arabidopsis thaliana
Author(s): Havlova, K (Havlova, Katerina); Dvorackova, M (Dvorackova, Martina); Peiro, R (Peiro, Ramon); Abia, D (Abia, David); Mozgova, I (Mozgova, Iva); Vansacova, L (Vansacova, Lenka); Gutierrez, C (Gutierrez, Crisanto); Fajkus, J (Fajkus, Jiri)
Source: PLANT MOLECULAR BIOLOGY **Volume:** 92 **Issue:** 4-5 **Pages:** 457-471 **DOI:** 10.1007/s11103-016-0524-1 **Published:** NOV 2016
Abstract: Approximately seven hundred 45S rRNA genes (rDNA) in the Arabidopsis thaliana genome are organised in two 4 Mbp-long arrays of tandem repeats arranged in head-to-tail fashion separated by an intergenic spacer (IGS). These arrays make up 5 % of the A. thaliana genome. IGS are rapidly evolving sequences and frequent rearrangements inside the rDNA loci have generated considerable interspecific and even intra-individual variability which allows to distinguish among otherwise highly conserved rRNA genes. The IGS has not been comprehensively described despite its potential importance in regulation of rDNA transcription and replication. Here we describe the detailed sequence variation in the complete IGS of A. thaliana WT plants and provide the reference/consensus IGS sequence, as well as genomic DNA analysis. We further investigate mutants dysfunctional in chromatin assembly factor-1 (CAF-1) (fas1 and fas2 mutants), which are known to have a reduced number of rDNA copies, and plant lines with restored CAF-1 function (segregated from a fas1xfas2 genetic background) showing major rDNA rearrangements. The systematic rDNA loss in CAF-1 mutants leads to the decreased variability of the IGS and to the occurrence of distinct IGS variants. We present for the first time a comprehensive and representative set of complete IGS sequences, obtained by conventional cloning and by Pacific Biosciences sequencing. Our data expands the knowledge of the A. thaliana IGS sequence arrangement and variability, which has not been available in full and in detail until now.

This is also the first study combining IGS sequencing data with RFLP analysis of genomic DNA.
Accession Number: WOS:000387114900005
PubMed ID: 27531496
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mozgova, Iva	J-5970-2017	0000-0002-3815-9223
Fajkus, Jiri	D-2499-2012	0000-0002-3112-1716
Gutierrez, Crisanto		0000-0001-8905-8222

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Record 218 of 491
Title: A theoretical study of intramolecular H-bonding and metal-ligand interactions in some complexes with bicyclic guanidine ligands
Author(s): Chahkandi, M (Chahkandi, Mohammad); Khoshbakht, BM (Khoshbakht, Behnaz Madani); Mirzaei, M (Mirzaei, Masoud)
Source: COMPUTATIONAL AND THEORETICAL CHEMISTRY **Volume:** 1095 **Pages:** 36-43 **DOI:** 10.1016/j.comptc.2016.09.014 **Published:** NOV 1 2016
Abstract: The reported complexes formulated as [MnCl2(hppH)(2)] (1), [FeCl2(hppH)(2)],(2), and [NiCl2(hppH)(2)] (3) and a new theoretically designed example, [CuCl2(hppH)(2)] (4), have been used for calculations at the B3LYP/ LANL2DZ/6-311G (d, p) level of density functional theory (DFT). The intramolecular hydrogen bonds (HB) N-H center dot center dot center dot Cl could followed through their physicochemical properties such as, vibrational frequency, electronic transmission in UV-Visible spectroscopy, metal-ligand donor-acceptor interactions in NBO analysis, total energy and frontier molecular orbital energy. These properties influenced by the relationship of structure and metal-ligand electron density exchange will be discussed. The computations revealed that the stronger N-H center dot center dot center dot Cl HB exists in complexes with longer M-Cl and M-N-imine bonds and shorter H center dot center dot center dot Cl bond, and vice versa that confirms the shortest and longest HBs in 4 and 3, respectively. These results agree with the second-order perturbation energies obtained by NBO analysis within charge transfer from the proton-acceptor chlorine to the p* orbital of the N atom. The calculated electronic absorption spectra by TD-DFT calculations show the larger Cl- to M2+ donation in 2 and 3 in comparison with I and 4 that confirms the stronger HB in 1 and 4 compared to 2 and 3. In order to find the basis set effect on the structure, vibrational frequencies, and electronic transitions, we use another basis set def2-TZVP includes polarization function for Mn element in complex 1. The obtained test results showed unremarkable differences between two basis sets LANL2DZ and def2-TZVP (cf. Figs. S2, S3 and Tables S1 and S2 in Supplementary Materials). (C) 2016 Elsevier B.V. All rights reserved.
Accession Number: WOS:000386404900005
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mirzaei, Masoud		0000-0002-7256-4601

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Record 219 of 491
Title: Genetic Analyses Suggest Separate Introductions of the Pine Pathogen Lecanosticta acicola Into Europe
Author(s): Janousek, J (Janousek, Josef); Wingfield, MJ (Wingfield, Michael J.); Monsivais, JGM (Monsivais, Jose G. Marmolejo); Jankovsky, L (Jankovsky, Libor); Stauffer, C (Stauffer, Christian); Konecny, A (Konecny, Adam); Barnes, I (Barnes, Irene)
Source: PHYTOPATHOLOGY **Volume:** 106 **Issue:** 11 **Pages:** 1413-1425 **DOI:** 10.1094/PHYTO-10-15-0271-R **Published:** NOV 2016
Abstract: Lecanosticta acicola is a heterothallic ascomycete that causes brown spot needle blight on native and nonnative Pinus spp. in many regions of the world. In this study we investigated the origin of European L. acicola populations and estimated the level of random mating of the pathogen in affected areas. Part of the elongation factor 1-alpha gene was sequenced, 11 microsatellite regions were screened, and the mating type idiomorphs were determined for 201 isolates of L. acicola collected from three continents and 17 host species. The isolates from Mexico and Guatemala were unique, highly diverse and could represent cryptic species of Lecanosticta. The isolates from East Asia formed a uniform and discrete group. Two distinct populations were identified in both North America and Europe. Approximate Bayesian computation analyses strongly suggest independent introductions of two populations from North America into Europe. Microsatellite data and mating type distributions indicated random recombination in the populations of North America and Europe. Its intercontinental introduction can most likely be explained as a consequence of the movement of infected plant material. In contrast, the spread of L. acicola within Europe appears to be primarily due to conidial dispersion and probably also ascospore dissemination.
Accession Number: WOS:000385900600021
PubMed ID: 26714104
ISSN: 0031-949X
eISSN: 1943-7684

Record 220 of 491
Title: Understanding radiation damage on sub-cellular scale using RADAMOL simulation tool
Author(s): Stepan, V (Stepan, Vaclav); Davidkova, M (Davidkova, Marie)
Source: RADIATION PHYSICS AND CHEMISTRY **Volume:** 128 **Pages:** 11-17 **DOI:** 10.1016/j.radphyschem.2016.06.031 **Published:** NOV 2016
Abstract: We present an overview of the biophysical model RADAMOL developed as a Monte Carlo simulation tool for physical, physico-chemical and chemical stages of ionizing radiation action. Direct and indirect radiation damage by 10 keV electrons, and protons and alpha particles with energies from 1 MeV up to 30 MeV to a free DNA oligomer or DNA in the complex with lac repressor protein is analyzed. The role of radiation type and energy, oxygen concentration and DNA interaction with proteins on yields and distributions of primary biomolecular damage is demonstrated and discussed. (C) 2016 Elsevier Ltd. All rights reserved.
Accession Number: WOS:000385325400003
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Stepan, Vaclav	G-7865-2014	0000-0002-7696-2877
Davidkova, Marie	G-7845-2014	

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Record 221 of 491
Title: Direct hydrodeoxygenation of phenol over carbon-supported Ru catalysts: A computational study
Author(s): Rubes, M (Rubes, Miroslav); He, J (He, Junjie); Nachtigall, P (Nachtigall, Petr); Bludsky, O (Bludsky, Ota)
Source: JOURNAL OF MOLECULAR CATALYSIS A-CHEMICAL **Volume:** 423 **Pages:** 300-307 **DOI:** 10.1016/j.molcata.2016.07.007 **Published:** NOV 2016
Abstract: Catalytic hydrodeoxygenation of phenol over graphene-supported Ru nanoparticles was investigated by means of periodic DFF calculations to propose a mechanism for the direct deoxygenation (DDO) pathway. The calculated interaction energies and activation barriers for the C-O scission on bare particle models of Ru/C catalysts are in good agreement with previous computational studies on the flat Ru(0001) surface and more realistic Ru surfaces with step edges and terraces. The results for graphene-supported Ru10Hx particles indicate that a model of the Ru/C catalyst with explicit hydrogens chemisorbed on the surface of metallic nanoparticle is essential for a complete understanding of the DDO process. (C) 2016 Elsevier By. All rights reserved.
Accession Number: WOS:000383827600035
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Nachtigall, Petr	A-6220-2013	0000-0002-1628-7275
He, Junjie	O-6825-2017	0000-0001-6447-7893
Bludsky, Ota	A-5659-2008	

ISSN: 1381-1169

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Record 222 of 491

Title: On calibration of stochastic and fractional stochastic volatility models

Author(s): Mrazek, M (Mrazek, Milan); Pospisil, J (Pospisil, Jan); Sobotka, T (Sobotka, Tomas)

Source: EUROPEAN JOURNAL OF OPERATIONAL RESEARCH **Volume:** 254 **Issue:** 3 **Pages:** 1036-1046 **DOI:** 10.1016/j.ejor.2016.04.033 **Published:** NOV 1 2016

Abstract: In this paper we study optimization techniques for calibration of stochastic volatility models to real market data. Several optimization techniques are compared and used in order to solve the nonlinear least squares problem arising in the minimization of the difference between the observed market prices and the model prices. To compare several approaches we use a popular stochastic volatility model firstly introduced by Heston (1993) and a more complex model with jumps in the underlying and approximative fractional volatility. Calibration procedures are performed on two main data sets that involve traded DAX index options. We show how well both models can be fitted to a given option price surface. The routines alongside models are also compared in terms of out-of-sample errors. For the calibration tasks without having a good knowledge of the market (e.g. a suitable initial model parameters) we suggest an approach of combining local and global optimizers. This way we are able to retrieve superior error measures for all considered tasks and models. (C) 2016 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Pospisil, Jan	D-3886-2013	0000-0002-4288-1614

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Record 223 of 491

Title: Molecular dynamics study of the growth of crystalline ZrO2

Author(s): Houska, J (Houska, Jiri)

Source: SURFACE & COATINGS TECHNOLOGY **Volume:** 304 **Pages:** 23-30 **DOI:** 10.1016/j.surfcoat.2016.07.004 **Published:** OCT 25 2016

Abstract: Thin films of ZrO2 are of high interest due to a wide range of useful technological properties. Previously, the plasma -assisted preparation of ZrO2 has been described in terms of extrinsic process parameters such as total pressure, oxygen partial pressure or discharge power. In this paper the growth of ZrO2 is studied by atom-by-atom molecular dynamics simulations, focused on intrinsic process parameters such as the energy and energy distribution function of arriving atoms. The results show how do the film densification, crystal nucleation and uninterrupted crystal growth depend not only on the energy delivered into the growing films (i) per fast atom (ion) or (ii) per any atom, but especially (iii) on the fraction of fast atoms in the particle flux and (iv) on the mass of fast atoms (Zr or O). In parallel, there is a clear effect of.the temperature on crystal nucleation, contrary to a very weak effect of the temperature on crystal growth. The results facilitate defining new synthesis pathways for ZrO2, and constitute phenomena which may be relevant for other coating materials (isostructural HfO2 at the first place) as well. (C) 2016 Published by Elsevier B.V.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houska, Jiri	B-9616-2016	0000-0002-4809-4128

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Record 224 of 491

Title: Sequence-dependent separation of trinucleotides by ion-interaction reversed-phase liquid chromatography A structure-retention study assisted by soft-modelling and molecular dynamics

Author(s): Mikulasek, K (Mikulasek, Kamil); Jaron, KS (Jaron, Kamil S.); Kulhanek, P (Kulhanek, Petr); Bittova, M (Bittova, Miroslava); Havlis, J (Havlis, Jan)

Source: JOURNAL OF CHROMATOGRAPHY A **Volume:** 1469 **Pages:** 88-95 **DOI:** 10.1016/j.chroma.2016.09.060 **Published:** OCT 21 2016

Abstract: We studied sequence-dependent retention properties of synthetic 5'-terminal phosphate absent trinucleotides containing adenine, guanine and thymine through reversed-phase liquid chromatography (RPLC) and QSRR modelling. We investigated the influence of separation conditions, namely mobile phase composition (ion interaction agent content, pH and organic constituent content), on sequence-dependent separation by means of ion-interaction RPLC (II-RPLC) using two types of models: experimental design-artificial neural networks (ED-ANN), and linear regression based on molecular dynamics data. The aim was to determine those properties of the above-mentioned analytes responsible for the retention dependence of the sequence.

Our results show that there is a deterministic relation between sequence and II-RPLC retention properties of the studied trinucleotides. Further, we can conclude that the higher the content of ion-interaction agent in the mobile phase, the more prominent these properties are. We also show that if we approximate the polar component of solvation energy in QSRR by the electrostatic work in transferring molecules from vacuum to water, and the non-polar component by the solvent accessible surface area, these parameters best describe the retention properties of trinucleotides. There are some exceptions to this finding, namely sequences 5'-NAN-3', 5'-ANN-3', 5'-TGN-3', 5'-NTA-3'and 5'-NGA-3' (N stands for generic nucleotide). Their role is still unknown, but since linear regression including these specific constellations showed a higher observable variance coverage than the model with only the basic descriptors, we may assume that solvent-analyte interactions are responsible for the exceptional behaviour of 5'-NAN-3' trinucleotides and some intramolecular interactions of neighbouring nucleobases for 5'-TGN-3', 5'-NTA-3'and 5'-NGA-3' trinucleotides. (C) 2016 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kulhanek, Petr	D-6884-2012	0000-0002-4152-6514

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Record 225 of 491

Title: Theoretical and Experimental Study on the Optoelectronic Properties of Nb3O7(OH) and Nb2O5 Photoelectrodes

Author(s): Khan, W (Khan, Wilayat); Betzler, SB (Betzler, Sophia B.); Sipr, O (Sipr, Ondrej); Ciston, J (Ciston, Jim); Blaha, P (Blaha, Peter); Scheu, C (Scheu, Christina); Minar, J (Minar, Jan)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 120 **Issue:** 41 **Pages:** 23329-23338 **DOI:** 10.1021/acs.jpcc.6b06391 **Published:** OCT 20 2016

Abstract: Nb3O7(OH) and Nb2O5 nanostructures are promising alternative materials to conventionally used oxides, e.g. TiO2, in the field of photoelectrodes in dye -sensitized solar cells and photoelectrochemical cells. Despite this important future application, some of their central electronic properties such as the density of states, band gap, and dielectric function are not well understood. In this work, we present combined theoretical and experimental studies on Nb3O7(OH) and H- Nb2O5 to elucidate their spectroscopic, electronic, and transport properties. The theoretical results were obtained within the framework of density functional theory based on the full potential linearized augmented plane wave method. In particular, we show that the position of the H atom in Nb3O7(OH) has an important effect on its electronic properties. To verify theoretical predictions, we measured electron energy-loss spectra (EELS) in the low loss region, as well as, the O-K and Nb-M-3 element-specific edges. These results are compared with corresponding theoretical EELS calculations and are discussed in detail. In addition, our calculations of thermoelectric conductivity show that Nb3O7(OH) has more suitable optoelectronic and transport properties for photochemical application than the calcined H-Nb2O5 phase.

Accession Number: WOS:000386107600003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Minar, Jan	O-3186-2013	0000-0001-9735-8479
Blaha, Peter	F-2847-2010	0000-0001-5849-5788

ISSN: 1932-7447

Record 226 of 491

Title: Ab initio density functional theory study on the atomic and electronic structure of GaP/Si(001) heterointerfaces

Author(s): Romanyuk, O (Romanyuk, O.); Supplie, O (Supplie, O.); Susi, T (Susi, T.); May, MM (May, M. M.); Hannappel, T (Hannappel, T.)

Source: PHYSICAL REVIEW B **Volume:** 94 **Issue:** 15 **Article Number:** 155309 **DOI:** 10.1103/PhysRevB.94.155309 **Published:** OCT 18 2016

Abstract: The atomic and electronic band structures of GaP/Si(001) heterointerfaces were investigated by ab initio density functional theory calculations. Relative total energies of abrupt interfaces and mixed interfaces with Si substitutional sites within a few GaP layers were derived. It was found that Si diffusion into GaP layers above the first interface layer is energetically unfavorable. An interface with Si/Ga substitution sites in the first layer above the Si substrate is energetically the most stable one in thermodynamic equilibrium. The electronic band structure of the epitaxial GaP/Si(001) heterostructure terminated by the (2 x 2) surface reconstruction consists of surface and interface electronic states in the common band gap of two semiconductors. The dispersion of the states is anisotropic and differs for the abrupt Si-Ga, Si-P, and mixed interfaces. Ga 2p, P 2p, and Si 2p core-level binding-energy shifts were computed for the abrupt and the lowest-energy heterointerface structures. Negative and positive core-level shifts due to heterovalent bonds at the interface are predicted for the abrupt Si-Ga and Si-P interfaces, respectively. The distinct features in the heterointerface electronic structure and in the core-level shifts open new perspectives in the experimental characterization of buried polar-on-nonpolar semiconductor heterointerfaces.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Supplie, Oliver	D-2404-2017	0000-0002-2424-7118
May, Matthias	H-8552-2013	0000-0002-1252-806X
Romanyuk, Oleksandr		0000-0003-0430-3706

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Record 227 of 491

Title: High-Frequency H-1 NMR Chemical Shifts of Sn-II and Pb-II Hydrides Induced by Relativistic Effects: Quest for Pb-II Hydrides

Author(s): Vicha, J (Vicha, Jan); Marek, R (Marek, Radek); Straka, M (Straka, Michal)

Source: INORGANIC CHEMISTRY **Volume:** 55 **Issue:** 20 **Pages:** 10302-10309 **DOI:** 10.1021/acs.inorgchem.6b01575 **Published:** OCT 17 2016

Abstract: The role of relativistic effects on H-1 NMR chemical shifts of Sn-II and Pb-II hydrides is investigated by using fully relativistic DFT calculations. The stability of possible Pb-II hydride isomers is studied together with their H-1 NMR chemical shifts, which are predicted in the high-frequency region, up to 90 ppm. These H-1 signals are dictated by sizable relativistic contributions due to spin orbit coupling at the heavy atom and can be as large as 80 ppm for a hydrogen atom bound to Pb-II. Such high-frequency H-1 NMR chemical shifts of Pb-II hydride resonances cannot be detected in the H-1 NMR spectra with standard experimental setup. Extended NMR spectral ranges are thus suggested for studies of Pb-II compounds. Modulation of spin orbit relativistic contribution to H-1 NMR chemical shift is found to be important also in the experimentally known Sn-II hydrides. Because the H-1 NMR chemical shifts were found to be rather sensitive to the changes in the coordination sphere of the central metal in both Sn-II and Pb-II hydrides, their application for structural investigation is suggested.

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PubMed ID: 27681471

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Straka, Michal	E-5246-2011	0000-0002-7857-4990
Vicha, Jan	D-8417-2012	0000-0003-3698-8236

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Record 228 of 491

Title: NEEMP: software for validation, accurate calculation and fast parameterization of EEM charges

Author(s): Racek, T (Racek, Tomas); Pazurikova, J (Pazurikova, Jana); Varekova, RS (Varekova, Radka Svobodova); Geidl, S (Geidl, Stanislav); Krenek, A (Krenek, Ales); Falginella, FL (Falginella, Francesco Luca); Horsky, V (Horsky, Vladimir); Hejret, V (Hejret, Vaclav); Koca, J (Koca, Jaroslav)

Source: JOURNAL OF CHEMINFORMATICS **Volume:** 8 **Article Number:** 57 **DOI:** 10.1186/s13321-016-0171-1 **Published:** OCT 17 2016

Abstract: Background: The concept of partial atomic charges was first applied in physical and organic chemistry and was later also adopted in computational chemistry, bioinformatics and chemoinformatics. The electronegativity equalization method (EEM) is the most frequently used approach for calculating partial atomic charges. EEM is fast and its accuracy is comparable to the quantum mechanical charge calculation method for which it was parameterized. Several EEM parameter sets for various types of molecules and QM charge calculation approaches have been published and new ones are still needed and produced. Methodologies for EEM parameterization have been described in a few articles, but a software tool for EEM parameterization and EEM parameter sets validation has not been available until now.

Results: We provide the software tool NEEMP (http://ncbr.muni.cz/NEEMP), which offers three main functionalities: EEM parameterization [via linear regression (LR) and differential evolution with local minimization (DE-MIN)]; EEM parameter set validation (i.e., validation of coverage and quality) and EEM charge calculation. NEEMP functionality is shown using a parameterization and a validation case study. The parameterization case study demonstrated that LR is an appropriate approach for smaller and homogeneous datasets and DE-MIN is a suitable solution for larger and heterogeneous datasets. The validation case study showed that EEM parameter set coverage and quality can still be problematic. Therefore, it makes sense to verify the coverage and quality of EEM parameter sets before their use, and NEEMP is an appropriate tool for such verification. Moreover, it seems from both case studies that new EEM parameterizations need to be performed and new EEM parameter sets obtained with high quality and coverage for key structural databases.

Conclusion: We provide the software tool NEEMP, which is to the best of our knowledge the only available software package that enables EEM parameterization and EEM parameter set validation. Additionally, its DE-MIN parameterization method is an innovative approach, developed by ourselves and first published in this work. In addition, we also prepared four high-quality EEM parameter sets tailored to ligand molecules.

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PubMed ID: 27803746

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Krenek, Ales	I-1311-2016	0000-0002-3395-3196
Horsky, Vladimir	A-7537-2017	0000-0002-9252-5386
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901

ISSN: 1758-2946

Record 229 of 491

Title: Population structure and dispersal routes of an invasive parasite, Fascioloides magna, in North America and Europe

Author(s): Juhasova, L (Juhasova, Ludmila); Kralova-Hromadova, I (Kralova-Hromadova, Ivica); Bazsalovicsova, E (Bazsalovicsova, Eva); Minarik, G (Minarik, Gabriel); Stefka, J (Stefka, Jan); Mikulicek, P (Mikulicek, Peter); Palkova, L (Palkova, Lenka); Pybus, M (Pybus, Margo)

Source: PARASITES & VECTORS **Volume:** 9 **Article Number:** 547 **DOI:** 10.1186/s13071-016-1811-z **Published:** OCT 13 2016

Abstract: Background: Fascioloides magna (Trematoda: Fasciolidae) is an important liver parasite of a wide range of free-living and domestic ruminants; it represents a remarkable species due to its large spatial distribution, invasive character, and potential to colonize new territories. The present study provides patterns of population genetic structure and admixture in F. magna across all enzootic regions in North America and natural foci in Europe, and infers migratory routes of the parasite on both continents.

Methods: In total, 432 individuals from five North American enzootic regions and three European foci were analysed by 11 microsatellite loci. Genetic data were evaluated by several statistical approaches: (i) the population genetic structure of F. magna was inferred using program STRUCTURE; (ii) the genetic interrelationships between populations were analysed by PRINCIPAL COORDINATES ANALYSIS; and (iii) historical dispersal routes in North America and recent invasion routes in Europe were explored using MIGRATE.

Results: The analysis of dispersal routes of the parasite in North America revealed west-east and south-north lineages that partially overlapped in the central part of the continent, where different host populations historically met. The exact origin of European populations of F. magna and their potential translocation routes were determined. Flukes from the first European focus, Italy, were related to F. magna from northern Pacific coast, while parasites from the Czech focus originated from south-eastern USA, particularly South Carolina.

The Danube floodplain forests (third and still expanding focus) did not display relationship with any North American population; instead the Czech origin of the Danube population was indicated. A serial dilution of genetic diversity along the dispersion route across central and eastern Europe was observed. The results of microsatellite analyses were compared to previously acquired outputs from mitochondrial haplotype data and correlated with past human-directed translocations and natural migration of the final cervid hosts of F. magna. Conclusions: The present study revealed a complex picture of the population genetic structure and interrelationships of North American and European populations, global distribution and migratory routes of F. magna and an origin of European foci.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Stefka, Jan	G-9267-2014	0000-0002-1283-9730

ISSN: 1756-3305

Record 230 of 491

Title: Multidimensional cloud latency monitoring and evaluation

Author(s): Tomanek, O (Tomanek, Ondrej); Mulinka, P (Mulinka, Pavol); Kencl, L (Kencl, Lukas)

Source: COMPUTER NETWORKS **Volume:** 107 **Special Issue:** SI **Pages:** 104-120 **DOI:** 10.1016/j.comnet.2016.06.011 **Part:** 1 **Published:** OCT 9 2016

Abstract: Measuring or evaluating performance of a Cloud service is a non-trivial and highly ambiguous task. We focus on Cloud-service latency from the user's point of view, and, to this end, utilize the multidimensional latency measurements obtained using an in-house designed active-probing platform, CLAudit, deployed across PlanetLab and Microsoft Azure datacenters. The multiple geographic Vantage Points, multiple protocol layers and multiple datacenter locations of CLAudit measurements allow us to pinpoint with great precision if, where and what kind of a particular latency-generating event has happened. We analyze and interpret measurements over two one-month time-intervals, one in 2013 and one in 2016. As these traces are large, an automated interpretation has been appended to the data-capture process. In summary, we demonstrate the utility of the multidimensional approach and document the differences in the measured Cloud-services latency over time. Our measurements data is publicly available and we encourage the research community to use it for verification and further studies. (C) 2016 Elsevier B.V. All rights reserved.

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Record 231 of 491

Title: Towards understanding the mechanism of action of antibacterial N-alkyl-3-hydroxypyridinium salts: Biological activities, molecular modeling and QSAR studies

Author(s): Dolezal, R (Dolezal, Rafael); Soukup, O (Soukup, Ondrej); Malinak, D (Malinak, David); Savedra, RML (Savedra, Ranylson M. L.); Marek, J (Marek, Jan); Dolezalova, M (Dolezalova, Marie); Pasdiorova, M (Pasdiorova, Marketa); Salajkova, S (Salajkova, Sarka); Korabecny, J (Korabecny, Jan); Honegr, J (Honegr, Jan); Ramalho, TC (Ramalho, Teodorico C.); Kuca, K (Kuca, Kamil)

Source: EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY **Volume:** 121 **Pages:** 699-711 **DOI:** 10.1016/j.ejmech.2016.05.058 **Published:** OCT 4 2016

Abstract: In this study, we have carried out a combined experimental and computational investigation to elucidate several bred-in-the-bone ideas standing out in rational design of novel cationic surfactants as antibacterial agents. Five 3-hydroxypyridinium salts differing in the length of N-alkyl side chain have been synthesized, analyzed by high performance liquid chromatography, tested for in vitro activity against a panel of pathogenic bacterial and fungal strains, computationally modeled in water by a SCRF B3LYP/6-311++G(d,p) method, and evaluated by a systematic QSAR analysis. Given the results of this work, the hypothesis suggesting that higher positive charge of the quaternary nitrogen should increase antimicrobial efficacy can be rejected since 3-hydroxyl group does increase the positive charge on the nitrogen but, simultaneously, it significantly derogates the antimicrobial activity by lowering the lipophilicity and by escalating the desolvation energy of the compounds in comparison with non-hydroxylated analogues. Herein, the majority of the prepared 3-hydroxylated substances showed notably lower potency than the parent pyridinium structures, although compound 8 with C-12 alkyl chain proved a distinctly better antimicrobial activity in submicromolar range. Focusing on this anomaly, we have made an effort to reveal the reason of the observed activity through a molecular dynamics simulation of the interaction between the bacterial membrane and compound 8 in GROMACS software. (C) 2016 Elsevier Masson SAS. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Honegr, Jan	B-4487-2010	0000-0002-9225-677X
Dolezal, Rafael	B-3956-2017	
Savedra, Ranylson	O-8477-2016	0000-0002-4809-577X
Ramalho, Teodorico	H-3204-2012	0000-0002-7324-1353
Benkova, Marketa		0000-0002-9196-9073

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Record 232 of 491

Title: The nature of the light variability of magnetic Of?p star HD 191612

Author(s): Krticka, J (Krticka, J.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 594 **Article Number:** A75 **DOI:** 10.1051/0004-6361/201629222 **Published:** OCT 2016

Abstract: Context. A small fraction of hot OBA stars host global magnetic fields with field strengths of the order of 0.1 10 kG. This leads to the creation of persistent surface structures (spots) in stars with sufficiently weak winds as a result of the radiative diffusion. These spots become evident in spectroscopic and photometric variability. This type of variability is not expected in stars with strong winds, where the wind inhibits the radiative diffusion. Therefore, a weak photometric variability of the magnetic Of?p star HD 191612 is attributed to the light absorption in the circumstellar clouds.

Aims. We study the nature of the photometric variability of HD 191612. We assume that the variability results from variable wind blanketing induced by surface variations of the magnetic field tilt and modulated by stellar rotation.

Methods. We used our global kinetic equilibrium (NLTE) wind models with radiative force determined from the radiative transfer equation in the comoving frame (CMF) to predict the stellar emergent flux. Our models describe the stellar atmosphere in a unified manner and account for the influence of the wind on the atmosphere. The models are calculated for different wind mass-loss rates to mimic the effect of magnetic field tilt on the emergent fluxes. We integrate the emergent fluxes over the visible stellar surface for individual rotational phases, and calculate the rotationally modulated light curve of HD 191612.

Results. The wind blanketing that varies across surface of HD 191612 is able to explain a part of the observed light variability in this star. The mechanism is able to operate even at relatively low mass-loss rates. The remaining variability is most likely caused by the flux absorption in circumstellar clouds.

Conclusions. The variable wind blanketing is an additional source of the light variability in massive stars. The presence of the rotational light variability may serve as a proxy for the magnetic field.

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Record 233 of 491

Title: Diversity and host specificity of coccidia (Apicomplexa: Eimeriidae) in native and introduced squirrel species

Author(s): Hofmannova, L (Hofmannova, Lada); Romeo, C (Romeo, Claudia); Stohanzlova, L (Stohanzlova, Lucie); Jirsova, D (Jirsova, Dagmar); Mazzamuto, MV (Mazzamuto, Maria Vittoria); Wauters, LA (Wauters, Lucas Armand); Ferrari, N (Ferrari, Nicola); Modry, D (Modry, David)

Source: EUROPEAN JOURNAL OF PROTISTOLOGY **Volume:** 56 **Pages:** 1-14 **DOI:** 10.1016/j.ejop.2016.04.008 **Published:** OCT 2016

Abstract: Introduction of alien species into new areas can have detrimental effects on native ecosystems and impact the native species. The present study aims to identify coccidia infecting native and introduced squirrels in Italy, to gain insight into possible transmission patterns and role of monoxenous coccidia in mediating the competition between alien and native hosts. We collected 540 faecal samples of native red squirrels, Sciurus vulgaris, invasive alien grey squirrels, S. carolinensis, and introduced Pallas's squirrels, Callosciurus erythraeus. Total prevalence of Eimeria spp. was 95.6% in S. vulgaris, 95.7% in S. carolinensis and only 4.1% in C. erythraeus. Morphological examination revealed 3 Eimeria morphotypes. Phylogenetic analyses of Eimeria DNA based on 18S, ITS, cox I markers displayed fairly distinct monophyletic clades in the microscopically indistinguishable E2 morphotype, proving indisputable distinction between the isolates from red and grey squirrels. Grey squirrels successfully introduced E. lancasterensis from their native range, but

this species does not spill over to native red squirrels. Similarly, there is no evidence for the transmission of E. sciurorum from red to grey squirrels. The possible transmission and the potential role of monoxenous coccidia in mediating the competition between native and invasive squirrels in Italy were not confirmed. (C) 2016 Elsevier GmbH. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Modry, David	G-7815-2014	
Ferrari, Nicola	E-6331-2013	0000-0001-8959-3495
Romeo, Claudia	D-5916-2017	0000-0002-5964-2847
Wauters, Lucas Armand		0000-0002-7012-9200

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Record 234 of 491

Title: Dependence of characteristics of MSiBCN (M = Ti, Zr, Hf) on the choice of metal element: Experimental and ab-initio study

Author(s): Houska, J (Houska, J.); Mares, P (Mares, P.); Simova, V (Simova, V.); Zuzjakova, S (Zuzjakova, S.); Cerstvy, R (Cerstvy, R.); Vlcek, J (Vlcek, J.)

Source: THIN SOLID FILMS **Volume:** 616 **Pages:** 359-365 **DOI:** 10.1016/j.tsf.2016.08.066 **Published:** OCT 1 2016

Abstract: The paper deals with MSiBCN (M = Ti, Zr, Hf) thin films prepared by pulsed dc reactive magnetron sputtering of M15Si20(B4C)(65) targets. We focus on the effect of M choice and N-2 + Ar discharge gas mixture composition. The experimental results are complemented and explained by ab-initio calculations. We find that the transition from Ti through Zr to Hf leads to (i) increasing driving force towards segregation, (ii) weaker role of M around the Fermi level and opening of a wider band gap in N-rich compositions, (iii) higher electrical resistivity and lower extinction-coefficient in N-rich compositions, (iv) increasing energy resulting from the oxidation of constituent M-containing phases, and consequently decreasing oxidation resistance of N-poor compositions and (v) increasing oxidation resistance of N-rich compositions. The results are important for the design of future coatings with tailored combinations of mechanical, electrical and optical properties and oxidation resistance. (C) 2016 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vlcek, Jaroslav	B-9259-2016	0000-0003-2627-2074
Cerstvy, Radomir	C-3767-2016	0000-0001-8507-6642
Houska, Jiri	B-9616-2016	0000-0002-4809-4128
Zuzjakova, Sarka	B-2035-2016	0000-0001-8140-192X

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Record 235 of 491

Title: The Evolution of the FT/TFL1 Genes in Amaranthaceae and Their Expression Patterns in the Course of Vegetative Growth and Flowering in Chenopodium rubrum

Author(s): Drabesova, J (Drabesova, Jana); Cerna, L (Cerna, Lucie); Masterova, H (Masterova, Helena); Kolouskova, P (Kolouskova, Pavla); Potocky, M (Potocky, Martin); Storchova, H (Storchova, Helena)

Source: G3-GENES GENOMES GENETICS **Volume:** 6 **Issue:** 10 **Pages:** 3065-3076 **DOI:** 10.1534/g3.116.028639 **Published:** OCT 2016

Abstract: The FT/TFL1 gene family controls important aspects of plant development: MFT-like genes affect germination, TFL1-like genes act as floral inhibitors, and FT-like genes are floral activators. Gene duplications produced paralogs with modified functions required by the specific lifestyles of various angiosperm species. We constructed the transcriptome of the weedy annual plant Chenopodium rubrum and used it for the comprehensive search for the FT/TFL1 genes. We analyzed their phylogenetic relationships across Amaranthaceae and all angiosperms. We discovered a very ancient phylogenetic clade of FT genes represented by the CrFTL3 gene of C. rubrum. Another paralog CrFTL2 showed an unusual structural rearrangement which might have contributed to the functional shift. We examined the transcription patterns of the FT/TFL1 genes during the vegetative growth and floral transition in C. rubrum to get clues about their possible functions. All the genes except for the constitutively expressed CrFTL2 gene, and the CrFTL3 gene, which was transcribed only in seeds, exhibited organ-specific expression influenced by the specific light regime. The CrFTL1 gene was confirmed as a single floral activator from the FT/TFL1 family in C. rubrum. Its floral promoting activity may be counteracted by CrTFL1. C. rubrum emerges as an easily manipulated model for the study of floral induction in weedy fast-cycling plants lacking a juvenile phase.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Potocky, Martin	B-7041-2008	0000-0002-3699-7549

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Record 236 of 491

Title: Artificial proteins as allosteric modulators of PDZ3 and SH3 in two-domain constructs: A computational characterization of novel chimeric proteins

Author(s): Kirubakaran, P (Kirubakaran, Palani); Pfeiferova, L (Pfeiferova, Lucie); Bousova, K (Bousova, Kristyna); Bednarova, L (Bednarova, Lucie); Obsilova, V (Obsilova, Veronika); Vondrasek, J (Vondrasek, Jiri)

Source: PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS **Volume:** 84 **Issue:** 10 **Pages:** 1358-1374 **DOI:** 10.1002/prot.25082 **Published:** OCT 2016

Abstract: Artificial multidomain proteins with enhanced structural and functional properties can be utilized in a broad spectrum of applications. The design of chimeric fusion proteins utilizing protein domains or one-domain miniproteins as building blocks is an important advancement for the creation of new biomolecules for biotechnology and medical applications. However, computational studies to describe in detail the dynamics and geometry properties of two-domain constructs made from structurally and functionally different proteins are lacking. Here, we tested an in silico design strategy using all-atom explicit solvent molecular dynamics simulations. The well-characterized PDZ3 and SH3 domains of human zonula occludens (ZO-1) (3TSZ), along with 5 artificial domains and 2 types of molecular linkers, were selected to construct chimeric two-domain molecules. The influence of the artificial domains on the structure and dynamics of the PDZ3 and SH3 domains was determined using a range of analyses. We conclude that the artificial domains can function as allosteric modulators of the PDZ3 and SH3 domains. Proteins 2016; 84:1358-1374. (c) 2016 Wiley Periodicals, Inc.

Accession Number: WOS:000383678800003

PubMed ID: 27273513

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Obsilova, Veronika	B-7116-2012	0000-0003-4887-0323
Palani, Kirubakaran		0000-0002-9749-729X

ISSN: 0887-3585

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Record 237 of 491

Title: The effect of chemical modification of DNA base on binding of Hg-II and Ag-I in metal-mediated base pairs

Author(s): Sebera, J (Sebera, Jakub); Tanaka, Y (Tanaka, Yoshiyuki); Ono, A (Ono, Akira); Sychrovsky, V (Sychrovsky, Vladimir)

Source: INORGANICA CHIMICA ACTA **Volume:** 452 **Special Issue:** SI **Pages:** 199-204 **DOI:** 10.1016/j.ica.2016.03.007 **Published:** OCT 1 2016

Abstract: The Gibbs free energy of formation of metallo-base pair was calculated for the base pairs composed of T, U, F, CN, C and I nucleosides and Hg-II and Ag-I metals. The effect of particular metal and the effect of pH on relative stabilization of metallo-base pairs were studied with calculated Gibbs free energies. The stability of Hg-mediated base pairs gradually decreased owing to the F and CN chemical modification of thymine at carbon C5 and owing to the imino to imidazole change of N3 nitrogen atom linked with Hg-II. The prevalence of Ag-I-stabilization versus Hg-II-stabilization was calculated for the metallo-base pairs composed of T, U, F, CN, C and I nucleosides where nucleophilicity of N3

nitrogen atom gradually decreased. The calculated relative stabilizations of metallo-base pairs agreed qualitatively with the increase in melting temperatures measured previously for respective duplexes upon adding Hg-II and Ag-I metals (Okamoto et al., 2009). The absolute magnitude of (1)J(Hg,N) and (2)J(N,N) coupling constants across metal-mediated linkage increased owing to F and CN modification of T and further increase of magnitudes off-couplings was calculated for imino to imidazole change of metal-bound nitrogen.

Accession Number: WOS:000385606600026

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Tanaka, Yoshiyuki	B-1730-2008	
Sebera, Jakub	B-6112-2013	0000-0001-5671-5206
Sychrovsky, Vladimir	G-5558-2014	

ISSN: 0020-1693

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Record 238 of 491

Title: Functional adaptation of crustacean exoskeletal elements through structural and compositional diversity: a combined experimental and theoretical study

Author(s): Fabritius, HO (Fabritius, Helge-Otto); Ziegler, A (Ziegler, Andreas); Friak, M (Friak, Martin); Nikolov, S (Nikolov, Svetoslav); Huber, J (Huber, Julia); Seidl, BHM (Seidl, Bastian H. M.); Ruangchai, S (Ruangchai, Sukhum); Alagboso, FI (Alagboso, Francisca I.); Karsten, S (Karsten, Simone); Lu, J (Lu, Jin); Janus, AM (Janus, Anna M.); Petrov, M (Petrov, Michal); Zhu, LF (Zhu, Li-Fang); Hemzalova, P (Hemzalova, Pavlina); Hild, S (Hild, Sabine); Raabe, D (Raabe, Dierk); Neugebauer, J (Neugebauer, Joerg)

Source: BIOINSPIRATION & BIOMIMETICS **Volume:** 11 **Issue:** 5 **Article Number:** 055006 **DOI:** 10.1088/1748-3190/11/5/055006 **Published:** OCT 2016

Abstract: The crustacean cuticle is a composite material that covers the whole animal and forms the continuous exoskeleton. Nano-fibers composed of chitin and protein molecules form most of the organic matrix of the cuticle that, at the macroscale, is organized in up to eight hierarchical levels. At least two of them, the exo- and endocuticle, contain a mineral phase of mainly Mg-calcite, amorphous calcium carbonate and phosphate. The high number of hierarchical levels and the compositional diversity provide a high degree of freedom for varying the physical, in particular mechanical, properties of the material. This makes the cuticle a versatile material ideally suited to form a variety of skeletal elements that are adapted to different functions and the eco-physiological strains of individual species. This review presents our recent analytical, experimental and theoretical studies on the cuticle, summarising at which hierarchical levels structure and composition are modified to achieve the required physical properties. We describe our multi-scale hierarchical modeling approach based on the results from these studies, aiming at systematically predicting the structure-composition-property relations of cuticle composites from the molecular level to the macro-scale. This modeling approach provides a tool to facilitate the development of optimized biomimetic materials within a knowledge-based design approach.

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PubMed ID: 27609556

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Petrov, Michal	R-8723-2017	0000-0002-8680-6317
Nikolov, Svetoslav		0000-0002-3760-804X

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Record 239 of 491

Title: Sensitivity of Lambda single-particle energies to the Lambda N spin-orbit coupling and to nuclear core structure in p-shell and sd-shell hypernuclei

Author(s): Vesely, P (Vesely, P.); Hiyama, E (Hiyama, E.); Hrtankova, J (Hrtankova, J.); Mares, J (Mares, J.)

Source: NUCLEAR PHYSICS A **Volume:** 954 **Pages:** 260-272 **DOI:** 10.1016/j.nuclphysa.2016.05.013 **Published:** OCT 2016

Abstract: We introduce a mean field model based on realistic 2-body baryon interactions and calculate spectra of a set of p-shell and sd-shell Lambda hypernuclei - C-13(Lambda), O-17(Lambda), Ne-21(Lambda), Si-29(Lambda) and Ca-41(Lambda). The hypernuclear spectra are compared with the results of a relativistic mean field (RMF) model and available experimental data. The sensitivity of Lambda single-particle energies to the nuclear core structure is explored. Special attention is paid to the effect of spin orbit Lambda N interaction on the energy splitting of the Lambda single particle levels 0p(3/2) and 0p(1/2). In particular, we analyze the contribution of the symmetric (SLS) and the anti-symmetric (ALS) spin-orbit terms to the energy splitting. We give qualitative predictions for the calculated hypernuclei. (C) 2016 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mares, Jiri	H-3387-2014	

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Record 240 of 491

Title: Calculation of Raman parameters of real-size zigzag (n, 0) single-walled carbon nanotubes using finite-size models

Author(s): Kupka, T (Kupka, Teobald); Stachow, M (Stachow, Michal); Stobinski, L (Stobinski, Leszek); Kaminsky, J (Kaminsky, Jakub)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 36 **Pages:** 25058-25069 **DOI:** 10.1039/c6cp04100k **Published:** SEP 28 2016

Abstract: Structural and selected Raman features of pristine single-walled carbon nanotubes (SWCTNs) with diameters from 0.4 to 1.2 nm and total lengths up to 2.15 nm were studied using the density functional theory (DFT) at the UB3LYP/6-31G* level. Models of different lengths (1, 4, 6 and 10 adjacent bamboo-units) of zigzag (n, 0) SWCNTs, for n ranging from 5 to 15, were studied. Highly systematic changes of individual CC bond lengths and angles along the nanotube axis were observed and described for the longest models. Predicted Raman active radial breathing mode (RBM) vibrational frequencies regularly decreased upon increasing the nanotube diameter and only a negligible effect of the tube length was observed. The changes in calculated RBM frequencies with increasing diameter were close to values estimated using empirical formulas. The experimental G-mode characteristics were reasonably well reproduced using the 4-unit model, especially for tubes with the diameter d > 1 nm. Raman features were also determined for cyclacenes representing the shortest models of SWCNTs. Calculated RBM frequencies of cyclacenes match closely the values for longer SWCNT models but are too inaccurate in the case of the G-mode. For the first time, the Raman properties of SWCNTs were also determined using the Cartesian coordinate tensor (CCT) transfer technique, thus providing reasonable frequencies of Raman active bands for long tubes consisting of 10 bamboo-units.

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PubMed ID: 27711454

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022
Kupka, Teobald		0000-0002-6252-3822

ISSN: 1463-9076

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Record 241 of 491

Title: Point defects stabilise cubic Mo-N and Ta-N

Author(s): Koutna, N (Koutna, Nikola); Holec, D (Holec, David); Svoboda, O (Svoboda, Ondrej); Klimashin, FF (Klimashin, Fedor F.); Mayrhofer, PH (Mayrhofer, Paul H.)

Source: JOURNAL OF PHYSICS D-APPLIED PHYSICS **Volume:** 49 **Issue:** 37 **Article Number:** 375303 **DOI:** 10.1088/0022-3727/49/37/375303 **Published:** SEP 21 2016

Abstract: We employ ab initio calculations to investigate energetics of point defects in metastable rocksalt cubic Ta-N and Mo-N. Our results reveal a strong tendency to off-stoichiometry, i.e. defected structures are surprisingly predicted to be more stable than perfect ones with 1 : 1 metal-to-nitrogen stoichiometry. Despite the similarity of Ta-N and Mo-N systems in exhibiting this unusual behaviour, we also point out their crucial differences. While Ta-N significantly favours metal vacancies, Mo-N exhibits similar energies of formation regardless of the vacancy type (V-Mo, V-N) as long as their concentration is below approximate to 15 at.%. The overall lowest energies of formation were obtained for Ta0.78N and Mo0.91N, which are hence predicted to be the most stable compositions. To account for various experimental conditions during synthesis, we further evaluated the

phase stability as a function of chemical potential of individual species. The proposed phase diagrams reveal four stable compositions, Mo0.84N, Mo0.91N, MoN0.69 and MoN0.44, in the case of Mo-N and nine stable compositions in the case of Ta-N indicating the important role of metal under-stoichiometry, since Ta0.75N and Ta0.78N significantly dominate the diagram. This is particularly important for understanding and designing experiments using non-equilibrium deposition techniques. Finally, we discuss the role of defect ordering and estimate a cubic lattice parameter as a function of defect contents and put them in the context of existing literature theoretical and experimental data.

Accession Number: WOS:000384093000022

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mayrhofer, Paul	A-9640-2011	0000-0001-7328-9333

ISSN: 0022-3727

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Record 242 of 491

Title: CenH3 evolution reflects meiotic symmetry as predicted by the centromere drive model

Author(s): Zedek, F (Zedek, Frantisek); Bures, P (Bures, Petr)

Source: SCIENTIFIC REPORTS **Volume:** 6 **Article Number:** 33308 **DOI:** 10.1038/srep33308 **Published:** SEP 15 2016

Abstract: The centromere drive model explaining rapid evolution of eukaryotic centromeres predicts higher frequency of positive selection acting on centromeric histone H3 (CenH3) in clades with asymmetric meiosis compared to the clades with only symmetric meiosis. However, despite the impression one might get from the literature, this key prediction of the centromere drive model has not only never been confirmed, but it has never been tested, because all the previous studies dealt only with the presence or absence instead of the frequency of positive selection. To provide evidence for or against different frequencies of positively selected CenH3 in asymmetrics and symmetrics, we have inferred the selective pressures acting on CenH3 in seventeen eukaryotic clades, including plants, animals, fungi, ciliates and apicomplexa, using codon-substitution models, and compared the inferred frequencies between asymmetrics and symmetrics in a quantitative manner. We have found that CenH3 has been evolving adaptively much more frequently in clades with asymmetric meiosis compared with clades displaying only symmetric meiosis which confirms the prediction of centromere drive model. Our findings indicate that the evolution of asymmetric meiosis required CenH3 to evolve adaptively more often to counterbalance the negative consequences of centromere drive.

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PubMed ID: 27629066

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zedek, Frantisek		0000-0003-1593-1775

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Record 243 of 491

Title: Electronic structure and magnetism of samarium and neodymium adatoms on free-standing graphene

Author(s): Kozub, AL (Kozub, Agnieszka L.); Shick, AB (Shick, Alexander B.); Maca, F (Maca, Frantisek); Kolorenc, J (Kolorenc, Jindrich); Lichtenstein, AI (Lichtenstein, Alexander I.)

Source: PHYSICAL REVIEW B **Volume:** 94 **Issue:** 12 **Article Number:** 125113 **DOI:** 10.1103/PhysRevB.94.125113 **Published:** SEP 8 2016

Abstract: The electronic structure of selected rare-earth atoms adsorbed on a free-standing graphene was investigated using methods beyond the conventional density functional theory (DFT+U, DFT+HIA, and DFT+ED). The influence of the electron correlations and the spin-orbit coupling on the magnetic properties has been examined. The DFT+U method predicts both atoms to carry local magnetic moments (spin and orbital) contrary to a nonmagnetic f(6) (J = 0) ground-state configuration of Sm in the gas phase. Application of DFT+Hubbard-I (HIA) and DFT+exact diagonalization (ED) methods cures this problem, and yields a nonmagnetic ground state with six f electrons and J = 0 for the Sm adatom. Our calculations show that Nd adatom remains magnetic, with four localized f electrons and J = 4.0. These conclusions could be verified by STM and XAS experiments.

Accession Number: WOS:000383238600006

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kozub, Agnieszka	M-3646-2015	0000-0001-6584-0201
Maca, Frantisek	G-4467-2014	
Shick, Alexander	C-1420-2013	0000-0003-2700-5517
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302

ISSN: 2469-9950

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Record 244 of 491

Title: Lattice energies of molecular solids from the random phase approximation with singles corrections

Author(s): Klimes, J (Klimes, Jiri)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 145 **Issue:** 9 **Article Number:** 094506 **DOI:** 10.1063/1.4962188 **Published:** SEP 7 2016

Abstract: We use the random phase approximation (RPA) method with the singles correlation energy contributions to calculate lattice energies of ten molecular solids. While RPA gives too weak binding, underestimating the reference data by 13.7% on average, much improved results are obtained when the singles are included at the GW singles excitations (GWSE) level, with average absolute difference to the reference data of only 3.7%. Consistently with previous results, we find a very good agreement with the reference data for hydrogen bonded systems, while the binding is too weak for systems where dispersion forces dominate. In fact, the overall accuracy of the RPA+GWSE method is similar to an estimated accuracy of the reference data. Published by AIP Publishing.

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PubMed ID: 27609003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Klimes, Jiri	D-8926-2011	0000-0003-4969-1343

ISSN: 0021-9606

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Record 245 of 491

Title: Defect-induced magnetic structure of CuMnSb

Author(s): Maca, F (Maca, F.); Kudrnovsky, J (Kudrnovsky, J.); Drchal, V (Drchal, V.); Turek, I (Turek, I.); Stelmakhovych, O (Stelmakhovych, O.); Beran, P (Beran, P.); Llobet, A (Llobet, A.); Marti, X (Marti, X.)

Source: PHYSICAL REVIEW B **Volume:** 94 **Issue:** 9 **Article Number:** 094407 **DOI:** 10.1103/PhysRevB.94.094407 **Published:** SEP 6 2016

Abstract: The observed ground state for the CuMnSb alloy is the antiferromagnetic (111) phase as confirmed by neutron diffraction experiments. Ab initio total energy calculations for ideal, defect-free CuMnSb contradict this result and indicate that other magnetic structures can have their total energies lower. It is known that Heusler alloys usually contain various defects depending on the sample preparation. We have therefore investigated magnetic phases of CuMnSb assuming the most common defects which exist in real experimental conditions. The full-potential supercell approach and a Heisenberg model approach using the coherent potential approximation are adopted. The results of the total energy supercell calculations indicate that defects that bring Mn atoms close together promote the antiferromagnetic (111) structure already for a low critical defect concentrations (approximate to 3%). A detailed study of exchange interactions between Mn moments further supports the above stabilization mechanism. Finally, the stability of the antiferromagnetic (111) order is enhanced by inclusion of electron correlations in narrow Mn bands. The present refinement structure analysis of the neutron scattering experiment supports theoretical conclusions.

Accession Number: WOS:000382718900007

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Beran, Premysl	F-8855-2012	0000-0002-1217-3131
Marti, Xavier	E-1103-2014	0000-0003-1653-5619
Maca, Frantisek	G-4467-2014	

ISSN: 2469-9950
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Record 246 of 491

Title: Stellar wind models of subluminous hot stars

Author(s): Krticka, J (Krticka, J.); Kubat, J (Kubat, J.); Krtickova, I (Krtickova, I.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 593 **Article Number:** A101 **DOI:** 10.1051/0004-6361/201628433 **Published:** SEP 2016

Abstract: Context. Mass-loss rate is one of the most important stellar parameters. Mass loss via stellar winds may influence stellar evolution and modifies stellar spectrum. Stellar winds of subluminous hot stars, especially subdwarfs, have not been studied thoroughly.
Aims. We aim to provide mass-loss rates as a function of subdwarf parameters and to apply the formula for individual subdwarfs, to predict the wind terminal velocities, to estimate the influence of the magnetic field and X-ray ionization on the stellar wind, and to study the interaction of subdwarf wind with mass loss from Be and cool companions.
Methods. We used our kinetic equilibrium (NLTE) wind models with the radiative force determined from the radiative transfer equation in the comoving frame (CMF) to predict the wind structure of subluminous hot stars. Our models solve stationary hydrodynamical equations, that is the equation of continuity, equation of motion, and energy equation and predict basic wind parameters.
Results. We predicted the wind mass-loss rate as a function of stellar parameters, namely the stellar luminosity, effective temperature, and metallicity. The derived wind parameters (mass-loss rates and terminal velocities) agree with the values derived from the observations. The radiative force is not able to accelerate the homogeneous wind for stars with low effective temperatures and high surface gravities. We discussed the properties of winds of individual subdwarfs. The X-ray irradiation may inhibit the flow in binaries with compact components. In binaries with Be components, the winds interact with the disk of the Be star.
Conclusions. Stellar winds exist in subluminous stars with low gravities or high effective temperatures. Despite their low mass-loss rates, they are detectable in the ultraviolet spectrum and cause X-ray emission. Subdwarf stars may lose a significant part of their mass during the evolution. The angular momentum loss in magnetic subdwarfs with wind may explain their low rotational velocities. Stellar winds are especially important in binaries, where they may be accreted on a compact or cool companion.

Accession Number: WOS:000385820100068

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kubat, Jiri	G-9032-2014	0000-0003-4269-8278

ISSN: 1432-0746

Record 247 of 491

Title: The Role of Retrotransposons in Gene Family Expansions in the Human and Mouse Genomes

Author(s): Janousek, V (Janousek, Vaclav); Laukaitis, CM (Laukaitis, Christina M.); Yanchukov, A (Yanchukov, Alexey); Karn, RC (Karn, Robert C.)

Source: GENOME BIOLOGY AND EVOLUTION **Volume:** 8 **Issue:** 9 **Pages:** 2632-2650 **DOI:** 10.1093/gbe/evw192 **Published:** SEP 2016

Abstract: Retrotransposons comprise a large portion of mammalian genomes. They contribute to structural changes and more importantly to gene regulation. The expansion and diversification of gene families have been implicated as sources of evolutionary novelties. Given the roles retrotransposons play in genomes, their contribution to the evolution of gene families warrants further exploration. In this study, we found a significant association between two major retrotransposon classes, LINEs and LTRs, and lineage-specific gene family expansions in both the human and mouse genomes. The distribution and diversity differ between LINEs and LTRs, suggesting that each has a distinct involvement in gene family expansion. LTRs are associated with open chromatin sites surrounding the gene families, supporting their involvement in gene regulation, whereas LINEs may play a structural role promoting gene duplication. Our findings also suggest that gene family expansions, especially in the mouse genome, undergo two phases. The first phase is characterized by elevated deposition of LTRs and their utilization in reshaping gene regulatory networks. The second phase is characterized by rapid gene family expansion due to continuous accumulation of LINEs and it appears that, in some instances at least, this could become a runaway process. We provide an example in which this has happened and we present a simulation supporting the possibility of the runaway process. Altogether we provide evidence of the contribution of retrotransposons to the expansion and evolution of gene families. Our findings emphasize the putative importance of these elements in diversification and adaptation in the human and mouse lineages.

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PubMed ID: 27503295

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Yanchukov, Alexey	A-2501-2014	0000-0002-9613-8770

ISSN: 1759-6653

Record 248 of 491

Title: Phylogenetic marker development for target enrichment from transcriptome and genome skim data: the pipeline and its application in southern African Oxalis (Oxalidaceae)

Author(s): Schmickl, R (Schmickl, Roswitha); Liston, A (Liston, Aaron); Zeisek, V (Zeisek, Vojtech); Oberlander, K (Oberlander, Kenneth); Weitemier, K (Weitemier, Kevin); Straub, SCK (Straub, Shannon C. K.); Cronn, RC (Cronn, Richard C.); Dreyer, LL (Dreyer, Leanne L.); Suda, J (Suda, Jan)

Source: MOLECULAR ECOLOGY RESOURCES **Volume:** 16 **Issue:** 5 **Special Issue:** SI **Pages:** 1124-1135 **DOI:** 10.1111/1755-0998.12487 **Published:** SEP 2016

Abstract: Phylogenetics benefits from using a large number of putatively independent nuclear loci and their combination with other sources of information, such as the plastid and mitochondrial genomes. To facilitate the selection of orthologous low-copy nuclear (LCN) loci for phylogenetics in nonmodel organisms, we created an automated and interactive script to select hundreds of LCN loci by a comparison between transcriptome and genome skim data. We used our script to obtain LCN genes for southern African Oxalis (Oxalidaceae), a speciose plant lineage in the Greater Cape Floristic Region. This resulted in 1164 LCN genes greater than 600bp. Using target enrichment combined with genome skimming (Hyb-Seq), we obtained on average 1141 LCN loci, nearly the whole plastid genome and the nrDNA cistron from 23 southern African Oxalis species. Despite a wide range of gene trees, the phylogeny based on the LCN genes was very robust, as retrieved through various gene and species tree reconstruction methods as well as concatenation. Cytonuclear discordance was strong. This indicates that organellar phylogenies alone are unlikely to represent the species tree and stresses the utility of Hyb-Seq in phylogenetics.

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PubMed ID: 26577756

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Schmickl, Roswitha	H-1624-2014	0000-0002-0632-5143
Zeisek, Vojtech	C-1240-2009	0000-0003-3481-9367
Dreyer, Leanne		0000-0001-7579-1028
Weitemier, Kevin		0000-0002-5793-0343
Cronn, Richard		0000-0001-5342-3494

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Record 249 of 491

Title: Room-temperature spin-orbit torque in NiMnSb

Author(s): Ciccarelli, C (Ciccarelli, C.); Anderson, L (Anderson, L.); Tshitoyan, V (Tshitoyan, V.); Ferguson, AJ (Ferguson, A. J.); Gerhard, F (Gerhard, F.); Gould, C (Gould, C.); Molenkamp, LW (Molenkamp, L. W.); Gayles, J (Gayles, J.); Zelezny, J (Zelezny, J.); Smejkal, L (Smejkal, L.); Yuan, Z (Yuan, Z.); Sinova, J (Sinova, J.); Freimuth, F (Freimuth, F.); Jungwirth, T (Jungwirth, T.)

Source: NATURE PHYSICS **Volume:** 12 **Issue:** 9 **Pages:** 855-860 **DOI:** 10.1038/NPHYS3772 **Published:** SEP 2016

Abstract: Materials that crystallize in diamond-related lattices, with Si and GaAs as their prime examples, are at the foundation of modern electronics. Simultaneously, inversion asymmetries in their crystal structure and relativistic spin-orbit coupling led to discoveries of non-equilibrium spin-polarization phenomena that are now extensively explored as an electrical means for manipulating magnetic moments in a variety of spintronic structures. Current research of these relativistic spin-orbit torques focuses primarily on magnetic transition-metal multilayers. The low-temperature diluted magnetic semiconductor (Ga,Mn)As, in which spin-orbit torques were initially discovered, has so far remained the only example showing the phenomenon among bulk non-centrosymmetric ferromagnets. Here we present a general framework, based on the complete set of crystallographic point groups, for identifying the potential presence and symmetry of spin-orbit torques in non-centrosymmetric crystals. Among the candidate room-temperature ferromagnets we chose to use NiMnSb, which is a member of the broad family of magnetic Heusler compounds. By performing all-electrical ferromagnetic resonance measurements in single-crystal epilayers of NiMnSb we detect room-temperature spin-orbit torques generated by effective fields of the expected symmetry and of a magnitude consistent with our ab initio calculations.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Gayles, Jacob	S-6348-2017	
Sinova, Jairo	G-9071-2014	0000-0002-9490-2333
Zelezny, Jakub	G-5276-2014	0000-0001-9471-0078
Yuan, Zhe	H-4018-2011	0000-0002-1898-7857
Freimuth, Frank		0000-0001-6193-5991
Ciccarelli, Chiara		0000-0003-2299-3704
Brune, Felicitas		0000-0003-0907-8202

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Record 250 of 491

Title: Exploring the thermoelectric and magnetic properties of uranium selenides: Tl2Ag2USe4 and Tl3Cu4USe6

Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Din, HU (Din, Haleem Ud); Khenata, R (Khenata, Rabah); Goumri-Said, S (Goumri-Said, Souraya)

Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 413 **Pages:** 57-64 **DOI:** 10.1016/j.jmmm.2016.03.073 **Published:** SEP 1 2016

Abstract: The electronic, magnetic and thermoelectric properties of Tl2Ag2USe4 and Tl3Cu4USe6 compounds were investigated using the full potential linear augmented plane wave (FP-LAPW) method based on the density functional theory (DFT). The exchange correlation was treated with the generalized gradient approximation plus optimized effective Hubbard parameter and spin orbit coupling (GGA+ U +SOC). The present uranium selenides show narrow direct energy band gap values of 0.7 and 0.875 eV for Tl2Ag2USe4 and Tl3Cu4USe6 respectively. For both selenides U-d/f states are responsible for electrical transport properties. Uranium atoms were the most contributors in the magnetic moment compared to other atoms and show ferromagnetic nature. The spin density isosurfaces show the polarization of neighboring atoms of Uranium, such as silver/copper and selenium. Thermoelectric calculations reveal that Tl3Cu4USe6 is more suitable for thermoelectric device applications than Tl2Ag2USe4. (C) 2016 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Azam, Sikander		0000-0001-5923-1127

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Page 6 (Records 251 -- 300)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 251 of 491

Title: Structure and genome release of Twort-like Myoviridae phage with a double-layered baseplate

Author(s): Novacek, J (Novacek, Jiri); Siborova, M (Siborova, Marta); Benesik, M (Benesik, Martin); Pantucek, R (Pantucek, Roman); Doskar, J (Doskar, Jiri); Plevka, P (Plevka, Pavel)

Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA **Volume:** 113 **Issue:** 33 **Pages:** 9351-9356 **DOI:** 10.1073/pnas.1605883113 **Published:** AUG 16 2016

Abstract: Bacteriophages from the family Myoviridae use double-layered contractile tails to infect bacteria. Contraction of the tail sheath enables the tail tube to penetrate through the bacterial cell wall and serve as a channel for the transport of the phage genome into the cytoplasm. However, the mechanisms controlling the tail contraction and genome release of phages with "double-layered" baseplates were unknown. We used cryo-electron microscopy to show that the binding of the Twort-like phage phi812 to the Staphylococcus aureus cell wall requires a 210 degrees rotation of the heterohexameric receptor-binding and tripod protein complexes within its baseplate about an axis perpendicular to the sixfold axis of the tail. This rotation reorients the receptor-binding proteins to point away from the phage head, and also results in disruption of the interaction of the tripod proteins with the tail sheath, hence triggering its contraction. However, the tail sheath contraction of Myoviridae phages is not sufficient to induce genome ejection. We show that the end of the phi812 double-stranded DNA genome is bound to one protein subunit from a connector complex that also forms an interface between the phage head and tail. The tail sheath contraction induces conformational changes of the neck and connector that result in disruption of the DNA binding. The genome penetrates into the neck, but is stopped at a bottleneck before the tail tube. A subsequent structural change of the tail tube induced by its interaction with the S. aureus cell is required for the genome's release.

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PubMed ID: 27469164

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Plevka, Pavel	H-8661-2014	0000-0003-4215-3315
Doskar, Jiri	O-1038-2017	
Pantucek, Roman	P-6758-2014	0000-0002-3950-675X

ISSN: 0027-8424

Record 252 of 491

Title: Phenanthrylene-butadiynylene and Phenanthrylene-thienylene Macrocycles: Synthesis, Structure, and Properties

Author(s): Phulwale, BV (Phulwale, Bhimrao Vaijnath); Mishra, SK (Mishra, Sushil Kumar); Necas, M (Necas, Marek); Mazal, C (Mazal, Ctibor)

Source: JOURNAL OF ORGANIC CHEMISTRY **Volume:** 81 **Issue:** 15 **Pages:** 6244-6252 **DOI:** 10.1021/acs.joc.6b00814 **Published:** AUG 5 2016

Abstract: A series of macrocycles consisting of 9,10-substituted phenanthrenes connected by butadiynylene linkers in positions 3 and 6 has been described as well as their transformation into the corresponding phenanthrylene-thienylene macrocycles. Structure and properties of the macrocycles, such as self-association in solution and optical and electrochemical properties, were studied and reported in a comparative manner with respect to the effects of the different sizes and shapes of the macrocycles and the character and length of their side chains.

Accession Number: WOS:000381236000010

PubMed ID: 27398717

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mazal, Ctibor	E-3293-2012	0000-0001-6815-4098
Necas, Marek	F-6833-2010	
Mishra, Sushil K.		0000-0002-3080-9754

ISSN: 0022-3263

Record 253 of 491

Title: Paralogues of nuclear ribosomal genes conceal phylogenetic signals within the invasive Asian fish tapeworm lineage: evidence from next generation sequencing data

Author(s): Brabec, J (Brabec, Jan); Kuchta, R (Kuchta, Roman); Scholz, T (Scholz, Tomas); Littlewood, DTJ (Littlewood, D. Timothy J.)

Source: INTERNATIONAL JOURNAL FOR PARASITOLOGY **Volume:** 46 **Issue:** 9 **Pages:** 555-562 **DOI:** 10.1016/j.ijpara.2016.03.009 **Published:** AUG 2016

Abstract: Complete mitochondrial genomes and nuclear rRNA operons of eight geographically distinct isolates of the Asian fish tapeworm Schyzocotyle acheilognathi (syn. Bothriocephalus acheilognathi), representing the parasite's global diversity spanning four continents, were fully characterised using an Illumina sequencing platform. This cestode species represents an extreme example of a highly invasive, globally distributed pathogen of veterinary importance with exceptionally low host specificity unseen elsewhere within the parasitic flatworms. In addition to eight specimens of S. acheilognathi, we fully characterised its closest known relative and the only congeneric species, Schyzocotyle nayarensis, from cyprinids in the Indian subcontinent. Since previous nucleotide sequence data on the Asian fish tapeworm were restricted to a single molecular locus of questionable phylogenetic utility-the nuclear rRNA genes -separating internal transcribed spacers-the mitogenomic data presented here offer a unique opportunity to gain the first detailed insights into both the intraspecific phylogenetic relationships and population genetic structure of the parasite, providing key baseline information for future research in the field. Additionally, we identify a previously unnoticed source of error and demonstrate the limited utility of the nuclear rRNA sequences, including the internal transcribed spacers that has likely misled most of the previous molecular phylogenetic and population genetic estimates on the Asian fish tapeworm. (C) 2016 Australian Society for Parasitology. Published by Elsevier Ltd. All rights reserved.

Accession Number: WOS:000381538000003

PubMed ID: 27155330

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Littlewood, Tim	B-5230-2008	0000-0002-2718-4001
Brabec, Jan	G-8419-2014	0000-0002-2636-414X
Scholz, Tomas	G-8360-2014	0000-0002-6340-3750
Kuchta, Roman	H-7828-2012	0000-0002-4219-6924

ISSN: 0020-7519

eISSN: 1879-0135

Record 254 of 491

Title: Estimation of Transition-Metal Empirical Parameters for Molecular Mechanical Force Fields

Author(s): Sebesta, F (Sebesta, Filip); Slama, V (Slama, Vladislav); Melcr, J (Melcr, Josef); Futera, Z (Futera, Zdenek); Burda, JV (Burda, Jaroslav V.)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 12 **Issue:** 8 **Pages:** 3681-3688 **DOI:** 10.1021/acs.jctc.6b00416 **Published:** AUG 2016

Abstract: Force-field parameters of the first row transition metals together with a few additional common elements such as those from the second (Rh, Ru) and third (Hg, Pt) rows of elements in ligated forms were determined based on the density functional theory calculations. Bonding characteristics were determined by averaging metal ligand force constants in optimal geometries from several chosen complexes of each metal in the most common oxidation numbers and structural arrangements. Parameters of Lennard-Jones potential were determined based on a supermolecular model. Our determined molecular mechanical parameters are compared with presently available parameters published by other groups. We performed two different kinds of testing in order to demonstrate the reliability of these parameters in the case of ligated metallo complexes. First, the nonbonding potential was constructed for, an additional set of 19 larger systems containing common complexes with organic molecules. The second test compares the Pt-O and Pt-H radial distribution functions for cisplatin in a box of TIP3P water with lately published studies.

Accession Number: WOS:000381320200025

PubMed ID: 27337427

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Burda, Jaroslav	C-9199-2009	0000-0001-9909-8797
Slama, Vladislav	Q-3330-2017	0000-0001-7339-5523
Futera, Zdenek	F-8771-2015	0000-0003-0471-8194

ISSN: 1549-9618
eISSN: 1549-9626

Record 255 of 491

Title: Modulating Electron Sharing in Ion-pi-Receptors via Substitution and External Electric Field: A Route toward Bond Strengthening
Author(s): Novak, M (Novak, Martin); Foroutan-Nejad, C (Foroutan-Nejad, Cina); Marek, R (Marek, Radek)
Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 12 **Issue:** 8 **Pages:** 3788-3795 **DOI:** 10.1021/acs.jctc.6b00586 **Published:** AUG 2016
Abstract: Substituted coronenes, a family of ion-pi receptors whose ion-affinities can be explained exclusively neither via ion-quadrupole nor induction/polarization mechanisms, are studied. The best descriptors of ion-affinity among these species are those characterizing charge-transfer between ions and the pi-systems, e.g. vertical ionization potential, electron affinity, and the relative energies of charge-transfer excited-states (CTESs). The variation of the electric multipole moments, polarizability, binding energy, and relative energy of CTESs in the presence of an external electric field (EEF) is evaluated. The results indicate that the EEF has a negligible effect on the polarizability and quadrupole moment of the systems. However, it significantly affects the binding energies, CTES energies, and the dipole moments of the receptors. Contrary to the changes in the dipole moment, the variation pattern of the binding energy is more consistent with the pattern observed for the CTES energy changes. Finally, by analyzing the exchange correlation component of the binding energy we demonstrate that the increased binding energy, i.e. bond strengthening, originates from enhanced electron sharing and multicenter covalency between the ions and the pi-systems as a result of the state-mixing between the ground-state and the CTESs. According to our findings, we hypothesize that the electron sharing and in extreme cases the multicenter covalency are the main driving forces for complexation of ions with extended pi-receptors such as carbon nanostructures.
Accession Number: WOS:000381320200035
PubMed ID: 27359252
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Novak, Martin	I-3248-2015	0000-0001-5067-1994
Marek, Radek	D-6929-2012	0000-0002-3668-3523

ISSN: 1549-9618
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Record 256 of 491

Title: Optoelectronic structure and related transport properties of BiCuSeO-based oxychalcogenides: First principle calculations
Author(s): Khan, W (Khan, Wilayat); Azam, S (Azam, Sikander); Kanoun, MB (Kanoun, Mohammed Benali); Goumri-Said, S (Goumri-Said, Souraya)
Source: SOLID STATE SCIENCES **Volume:** 58 **Pages:** 86-93 **DOI:** 10.1016/j.solidstatesciences.2016.05.012 **Published:** AUG 2016
Abstract: Recent experiments have revealed that the p-type BiCuSeO-based oxychalcogenides compounds exhibit a high thermoelectric figures of merit due to their very low lattice thermal conductivities and moderate Seebeck coefficient in the medium temperature range. In the present work, we reported on the optoelectronic and thermoelectric properties using the full potential linear augmented plane wave method and modified Becke-Johnson potential with spin-orbit coupling. The properties show that the BiCuSeO-based oxychalcogenides exhibit a semiconductor behavior with band gap values of 0.51, 0.45 and 0.41 eV for BiCuSO, BiCuSeO, and BiCuTeO, respectively. Due to their prominent role for thermoelectric applications, we combined Boltzmann transport theory to DFT results to compute the transport properties, mainly electronic conductivity, thermal conductivity, Seebeck coefficient and power factor. The present results show the dominance of BiCuTeO for thermoelectric application compared to the BiCuSO and BiCuSeO. (C) 2016 Elsevier Masson SAS. All rights reserved.
Accession Number: WOS:000381588100011
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Kanoun, Mohammed-Benali		0000-0002-2334-7889
Azam, Sikander		0000-0001-5923-1127

ISSN: 1293-2558
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Record 257 of 491

Title: Plant responses to ambient temperature fluctuations and water-limiting conditions: A proteome-wide perspective
Author(s): Johnova, P (Johnova, Patricie); Skalak, J (Skalak, Jan); Saiz-Fernandez, I (Saiz-Fernandez, Inigo); Brzobohaty, B (Brzobohaty, Bretislav)
Source: BIOCHIMICA ET BIOPHYSICA ACTA-PROTEINS AND PROTEOMICS **Volume:** 1864 **Issue:** 8 **Special Issue:** SI **Pages:** 916-931 **DOI:** 10.1016/j.bbapap.2016.02.007 **Published:** AUG 2016
Abstract: Background: Every year, environmental stresses such as limited water and nutrient availability, salinity, and temperature fluctuations inflict significant losses on crop yields across the globe. Recently, developments in analytical techniques, e.g. mass spectrometry, have led to great advances towards understanding how plants respond to environmental stresses. These processes are mediated by many molecular pathways and, at least partially, via proteome-environment interactions.
Scope of review: This review focuses on the current state of knowledge about interactions between the plant proteome and the environment, with a special focus on drought and temperature responses of plant proteome dynamics, and subcellular and organ-specific compartmentalization, in Arabidopsis thaliana and crop species.
Major conclusions: Correct plant development under non-optimal conditions requires complex self-protection mechanisms, many of them common to different abiotic stresses. Proteome analyses of plant responses to temperature and drought stresses have revealed an intriguing interplay of modifications, mainly affecting the photosynthetic machinery, carbohydrate metabolism, and ROS activation and scavenging. Imbalances between transcript-level and protein-level regulation observed during adaptation to abiotic stresses suggest that many of the regulatory processes are controlled at translational and post-translational levels; proteomics is thus essential in revealing important regulatory networks.
General significance: Because information from proteomic data extends far beyond what can be deduced from transcriptome analysis, the results of proteome studies have substantially deepened our understanding of stress adaptation in plants; this is clearly a prerequisite for designing strategies to improve the yield and quality of crops grown under unfavorable conditions brought about by ongoing climatic change.
This article is part of a Special Issue entitled: Plant Proteomics - a bridge between fundamental processes and crop production, edited by Dr. Hans-Peter Mock. (C) 2016 Elsevier B.V. All rights reserved.
Accession Number: WOS:000379276000005
PubMed ID: 26861773
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Saiz-Fernandez, Inigo	L-8255-2014	0000-0002-5907-1300

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Record 258 of 491

Title: Role of the proteome in phytohormonal signaling
Author(s): Cerny, M (Cerny, Martin); Novak, J (Novak, Jan); Habanova, H (Habanova, Hana); Cerna, H (Cerna, Hana); Brzobohaty, B (Brzobohaty, Bretislav)
Source: BIOCHIMICA ET BIOPHYSICA ACTA-PROTEINS AND PROTEOMICS **Volume:** 1864 **Issue:** 8 **Special Issue:** SI **Pages:** 1003-1015 **DOI:** 10.1016/j.bbapap.2015.12.008 **Published:** AUG 2016

Abstract: Phytohormones are orchestrators of plant growth and development A lot of time and effort has been invested in attempting to comprehend their complex signaling pathways but despite success in elucidating some key components, molecular mechanisms in the transduction pathways are far from being resolved. The last decade has seen a boom in the analysis of phytohormone-responsive proteins. Abscisic acid, auxin, brassinosteroids, cytokinin, ethylene, gibberellins, nitric oxide, oxylipins, strigolactones, salicylic acid - all have been analyzed to various degrees. For this review, we collected data from proteome-wide analyses resulting in a list of over 2000 annotated proteins from Arabidopsis proteomics and nearly 500 manually filtered protein families merged from all the data available from different species. We present the currently accepted model of phytohormone signaling, highlight the contributions made by proteomic-based research and describe the key nodes in phytohormone signaling networks, as revealed by proteome analysis. These include ubiguitination and proteasome mediated degradation, calcium ion signaling, redox homeostasis, and phosphoproteome dynamics. Finally, we discuss potential pitfalls and future perspectives in the field. This article is part of a Special Issue entitled: Plant Proteomics-a bridge between fundamental processes and crop production, edited by Dr. Hans-Peter Mock. (C) 2015 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cerny, Martin	D-7226-2012	
Novak, Jan	I-3635-2014	
Cerny, Martin		0000-0002-0651-4219

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Record 259 of 491

Title: Algorithms for computing strategies in two-player simultaneous move games

Author(s): Bosansky, B (Bosansky, Branislav); Lisy, V (Lisy, Viliam); Lanctot, M (Lanctot, Marc); Cermak, J (Cermak, Jiri); Winands, MHM (Winands, Mark H. M.)

Source: ARTIFICIAL INTELLIGENCE **Volume:** 237 **Pages:** 1-40 **DOI:** 10.1016/j.artint.2016.03.005 **Published:** AUG 2016

Abstract: Simultaneous move games model discrete, multistage interactions where at each stage players simultaneously choose their actions. At each stage, a player does not know what action the other player will take, but otherwise knows the full state of the game. This formalism has been used to express games in general game playing and can also model many discrete approximations of real-world scenarios. In this paper, we describe both novel and existing algorithms that compute strategies for the class of two-player zero-sum simultaneous move games. The algorithms include exact backward induction methods with efficient pruning, as well as Monte Carlo sampling algorithms. We evaluate the algorithms in two different settings: the offline case, where computational resources are abundant and closely approximating the optimal strategy is a priority, and the online search case, where computational resources are limited and acting quickly is necessary. We perform a thorough experimental evaluation on six substantially different games for both settings. For the exact algorithms, the results show that our pruning techniques for backward induction dramatically improve the computation time required by the previous exact algorithms. For the sampling algorithms, the results provide unique insights into their performance and identify favorable settings and domains for different sampling algorithms. (C) 2016 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Winands, Mark	L-3855-2014	0000-0002-0125-0824
Lisy, Viliam		0000-0002-1647-1507

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Record 260 of 491

Title: Lone-pair-pi interactions: analysis of the physical origin and biological implications

Author(s): Novotny, J (Novotny, Jan); Bazzi, S (Bazzi, Sophia); Marek, R (Marek, Radek); Kozelka, J (Kozelka, Jiri)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 28 **Pages:** 19472-19481 **DOI:** 10.1039/c6cp01524g **Published:** JUL 28 2016

Abstract: Lone-pair-pi (lp-pi) interactions have been suggested to stabilize DNA and protein structures, and to participate in the formation of DNA-protein complexes. To elucidate their physical origin, we have carried out a theoretical multi-approach analysis of two biologically relevant model systems, water-indole and water-uracil complexes, which we compared with the structurally similar chloride-tetracyanobenzene (TCB) complex previously shown to contain a strong charge-transfer (CT) binding component. We demonstrate that the CT component in lp-pi interactions between water and indole/uracil is significantly smaller than that stabilizing the Cl--TCB reference system. The strong lp(Cl-)-pi(TCB) orbital interaction is characterized by a small energy gap and an efficient lp-pi(star) overlap. In contrast, in lp-pi interactions between water and indole or uracil, the corresponding energy gap is larger and the overlap less efficient. As a result, water-uracil and water-indole interactions are weak forces composed by smaller contributions from all energy components: electrostatics, polarization, dispersion, and charge transfer. In addition, indole exhibits a negative electrostatic potential at its pi-face, making lp-pi interactions less favorable than O-H center dot center dot center dot pi hydrogen bonding. Consequently, some of the water-tryptophan contacts observed in X-ray structures of proteins and previously interpreted as lp-pi interactions [Luisi, et al., Proteins, 2004, 57, 1-8], might in fact arise from O-H center dot center dot center dot pi hydrogen bonding.

Accession Number: WOS:000379939100089

PubMed ID: 27411074

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Bazzi, Sophia		0000-0001-5885-3231

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Record 261 of 491

Title: Synergy between NMR measurements and MD simulations of protein/RNA complexes: application to the RRMs, the most common RNA recognition motifs

Author(s): Krepl, M (Krepl, Miroslav); Clery, A (Clery, Antoine); Blatter, M (Blatter, Markus); Allain, FHT (Allain, Frederic H. T.); Sponer, J (Sponer, Jiri)

Source: NUCLEIC ACIDS RESEARCH **Volume:** 44 **Issue:** 13 **Pages:** 6452-6470 **DOI:** 10.1093/nar/gkw438 **Published:** JUL 27 2016

Abstract: RNA recognition motif (RRM) proteins represent an abundant class of proteins playing key roles in RNA biology. We present a joint atomistic molecular dynamics (MD) and experimental study of two RRM-containing proteins bound with their single-stranded target RNAs, namely the Fox-1 and SRSF1 complexes. The simulations are used in conjunction with NMR spectroscopy to interpret and expand the available structural data. We accumulate more than 50 mu s of simulations and show that the MD method is robust enough to reliably describe the structural dynamics of the RRM-RNA complexes. The simulations predict unanticipated specific participation of Arg142 at the protein-RNA interface of the SRFS1 complex, which is subsequently confirmed by NMR and ITC measurements. Several segments of the protein-RNA interface may involve competition between dynamical local substates rather than firmly formed interactions, which is indirectly consistent with the primary NMR data. We demonstrate that the simulations can be used to interpret the NMR atomistic models and can provide qualified predictions. Finally, we propose a protocol for 'MD-adapted structure ensemble' as a way to integrate the simulation predictions and expand upon the deposited NMR structures. Unbiased mu s-scale atomistic MD could become a technique routinely complementing the NMR measurements of protein-RNA complexes.

Accession Number: WOS:000382999300041

PubMed ID: 27193998

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sponer, Jiri	D-9467-2012	
Krepl, Miroslav		0000-0002-9833-4281

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Record 262 of 491

Title: Modified Guanines as Constituents of Smart Ligands for Nucleic Acid Quadruplexes

Author(s): Durec, M (Durec, Matus); Zaccaria, F (Zaccaria, Francesco); Guerra, CF (Guerra, Celia Fonseca); Marek, R (Marek, Radek)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 22 **Issue:** 31 **Pages:** 10912-10922 **DOI:** 10.1002/chem.201601608 **Published:** JUL 25 2016

Abstract: Repetitive guanine-rich nucleic acid sequences play a crucial role in maintaining genome stability and the cell life cycle and represent potential targets for regulatory drugs. Recently, it has been demonstrated that guanine-based ligands with a porphyrin core can be used as markers of G-quadruplex assemblies in cell tissues. Herein, model systems of guanine-based ligands are explored by DFT methods. The energies of formation of modified guanine tetrads and those of modified tetrads stacked on the top of natural guanine tetrads have been calculated. The interaction energy has been decomposed into contributions from hydrogen bonding, stacking, and ion coordination and a twist-rise potential energy scan has been performed to find the individual local minima. Energy decomposition analysis reveals the impact of various substituents (F, Cl, Br, I, Me, NMe2) on individual energy terms. In addition, cooperative reinforcement in forming the modified and stacked tetrads, as well as the frontier orbitals participating in the hydrogenbonding framework involving the HOMO-LUMO gap between the occupied sigma(HOMO) on the proton-accepting C=O and =N- groups and unoccupied sigma(LUMO) on the N-H groups, has been studied. The investigated systems are demonstrated to have a potential in ligand development, mainly due to stacking enhancement compared with natural guanine, which is used as a reference.

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PubMed ID: 27385491

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fonseca Guerra, Celia	E-8851-2011	
Durec, Matus	D-9478-2012	0000-0001-9896-610X
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Fonseca Guerra, Celia		0000-0002-2973-5321

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Record 263 of 491

Title: The effect of the zeolite pore size on the Lewis acid strength of extra-framework cations

Author(s): Thang, HV (Ho Viet Thang); Frolich, K (Frolich, Karel); Shamzhy, M (Shamzhy, Mariya); Eliasova, P (Eliasova, Pavla); Rubes, M (Rubes, Miroslav); Cejka, J (Cejka, Jiri); Bulanek, R (Bulanek, Roman); Nachtigall, P (Nachtigall, Petr)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 27 **Pages:** 18063-18073 **DOI:** 10.1039/c6cp03343a **Published:** JUL 21 2016

Abstract: The catalytic activity and the adsorption properties of zeolites depend on their topology and composition. For a better understanding of the structure-activity relationship it is advantageous to focus just on one of these parameters. Zeolites synthesized recently by the ADOR protocol offer a new possibility to investigate the effect of the channel diameter on the adsorption and catalytic properties of zeolites: UTL, OKO, and PCR zeolites consist of the same dense 2D layers (IPC-1P) that are connected with different linkers (D4R, S4R, O-atom, respectively) resulting in the channel systems of different sizes (14R x 12R, 12R x 10R, 10R x 8R, respectively). Consequently, extra-framework cation sites compensating charge of framework Al located in these dense 2D layers (channel-wall sites) are the same in all three zeolites. Therefore, the effect of the zeolite channel size on the Lewis properties of the cationic sites can be investigated independent of other factors determining the quality of Lewis sites. UTL, OKO, and PCR and pillared 2D IPC-1PI materials were prepared in Li-form and their properties were studied by a combination of experimental and theoretical methods. Qualitatively different conclusions are drawn for Li+ located at the channel-wall sites and at the intersection sites (Li+ located at the intersection of two zeolite channels): the Lewis acid strength of Li+ at intersection sites is larger than that at channel-wall sites. The Lewis acid strength of Li+ at channel-wall sites increases with decreasing channel size. When intersecting channels are small (10R x 8R in PCR) the intersection Li+ sites are no longer stable and Li+ is preferentially located at the channel-wall sites. Last but not least, the increase in adsorption heats with the decreasing channel size (due to enlarged dispersion contribution) is clearly demonstrated.

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PubMed ID: 27326803

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Eliasova, Pavla	F-5300-2014	0000-0002-9473-8414
Cejka, Jiri	B-1833-2013	0000-0003-1400-1031
Shamzhy, Mariya	F-5477-2014	
Nachtigall, Petr	A-6220-2013	0000-0002-1628-7275
Thang, Ho Viet		0000-0002-8608-8941

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Record 264 of 491

Title: Conserving approximations for response functions of the Fermi gas in a random potential

Author(s): Janis, V (Janis, Vaclav); Kolorenc, J (Kolorenc, Jindrich)

Source: EUROPEAN PHYSICAL JOURNAL B **Volume:** 89 **Issue:** 7 **Article Number:** 170 **DOI:** 10.1140/epjb/e2016-70188-1 **Published:** JUL 20 2016

Abstract: One- and two-electron Green functions are simultaneously needed to determine the response functions of the electron gas in a random potential. Reliable approximations must retain consistency between the two types of Green functions expressed via Ward identities so that their output is compliant with macroscopic symmetries and conservation laws. Such a consistency is not directly guaranteed when summing nonlocal corrections to the local (dynamical) mean field. We analyze the reasons for this failure and show how the full Ward identity can generically be implemented in the diagrammatic approach to the vertex functions without breaking the analytic properties of the self-energy. We use the low-energy asymptotics of the conserving two-particle vertex determining the singular part of response and correlation functions to derive an exact representation of the diffusion constant in terms of Green functions of the perturbation theory. We then calculate explicitly the leading vertex corrections to the mean-field diffusion constant due to maximally-crossed diagrams.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302
Janis, Vaclav	A-8379-2011	0000-0001-5959-6935

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Record 265 of 491

Title: Interactions of the "piano-stool" [ruthenium(II)((6)-arene)(quinolone)Cl](+) complexes with water; DFT computational study

Author(s): Zabojnikova, T (Zabojnikova, Tereza); Cajzl, R (Cajzl, Radim); Kljun, J (Kljun, Jakob); Chval, Z (Chval, Zdenek); Turel, I (Turel, Iztok); Burda, JV (Burda, Jaroslav V.)

Source: JOURNAL OF COMPUTATIONAL CHEMISTRY **Volume:** 37 **Issue:** 19 **Pages:** 1766-1780 **DOI:** 10.1002/jcc.24373 **Published:** JUL 15 2016

Abstract: Full optimizations of stationary points along the reaction coordinate for the hydration of several quinolone Ru(II) half-sandwich complexes were performed in water environment using the B3PW91/6-31+G(d)/PCM/UAKS method. The role of diffuse functions (especially on oxygen) was found crucial for correct geometries along the reaction coordinate. Single-point (SP) calculations were performed at the B3LYP/6-311++G(2df,2pd)/DPCM/saled-UAKS level. In the first part, two possible reaction mechanismsassociative and dissociative were compared. It was found that the dissociative mechanism of the hydration process is kinetically slightly preferred. Another important conclusion concerns the reaction channels. It was found that substitution of chloride ligand (abbreviated in the text as dechlorination reaction) represents energetically and kinetically the most feasible pathway. In the second part the same hydration reaction was explored for reactivity comparison of the Ru(II)-complexes with several derivatives of nalidixic acid: cinoxacin, ofloxacin, and (thio)nalidixic acid. The hydration process is about four orders of magnitude faster in a basic solution compared to neutral/acidic environment with cinoxacin and nalidixic acid as the most reactive complexes in the former and latter environments, respectively. The explored hydration reaction is in all cases endergonic; nevertheless the endergonicity is substantially lower (by approximate to 6 kcal/mol) in basic environment. (c) 2016 Wiley Periodicals, Inc.

Accession Number: WOS:000379161900002
PubMed ID: 27185047
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Burda, Jaroslav	C-9199-2009	0000-0001-9909-8797
Chval, Zdenek	D-8964-2016	0000-0003-1922-8390
Cajzl, Radim		0000-0002-0192-6775

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Record 266 of 491
Title: Interpreting the Paramagnetic NMR Spectra of Potential Ru(III) Metallodrugs: Synergy between Experiment and Relativistic DFT Calculations
Author(s): Novotny, J (Novotny, Jan); Sojka, M (Sojka, Martin); Komorovsky, S (Komorovsky, Stanislav); Necas, M (Necas, Marek); Marek, R (Marek, Radek)
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 138 **Issue:** 27 **Pages:** 8432-8445 **DOI:** 10.1021/jacs.6b02749 **Published:** JUL 13 2016
Abstract: Ruthenium-based compounds are potential candidates for use as anticancer metallodrugs. The central ruthenium atom can be in the oxidation state +2 (e.g., RAPTA, RAED) or +3 (e.g., NAMI, 10). In this study we focus on paramagnetic NAMI analogs of a general structure [4-R-pyH](+)trans-[(RuCl4)-Cl-III(DMSO)(4-R-py)](-), where 4-R-py stands for a 4-substituted pyridine. As paramagnetic systems are generally considered difficult to characterize in detail by NMR spectroscopy, we performed a systematic structural and methodological NMR study of complexes containing variously substituted pyridines. The effect of the paramagnetic nature of these complexes on the H-1 and C-13 NMR chemical shifts was systematically investigated by temperature-dependent NMR experiments and density-functional theory (DFT) calculations. To understand the electronic factors influencing the orbital (delta(orb), temperature independent) and paramagnetic (delta(para), temperature-dependent) contributions to the total NMR chemical shifts, a relativistic two component DFT approach was used. The paramagnetic contributions to the C-13 NMR chemical shifts are correlated with the distribution of spin density in the ligand moiety and the C-13 isotropic hyperfine coupling constants, A(iso)(C-13), for the individual carbon atoms. To analyze the mechanism of spin distribution in the ligand, the contributions of molecular spin orbitals (MSOs) to the hyperfine coupling constants and the spatial distribution of the z-component of the spin density in the MSOs calculated at the relativistic four-component DFT level are discussed and rationalized. The significant effects of the substituent and the solvent on delta(para), particularly the contact contribution, are demonstrated. This work should contribute to further understanding of the link between the electronic structure and the NMR chemical shifts in open-shell systems, including the ruthenium-based metallodrugs investigated in this account.
Accession Number: WOS:000379794400026
PubMed ID: 27312929
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Necas, Marek	F-6833-2010	
Novotny, Jan	D-7676-2012	0000-0002-1203-9549
Komorovsky, Stanislav	N-4332-2016	0000-0002-5317-7200
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Sojka, Martin		0000-0001-5266-3963

ISSN: 0002-7863

Record 267 of 491
Title: Three-dimensional homologymodel of GlcNAc-TV glycosyltransferase
Author(s): Janos, P (Janos, Pavel); Kozmon, S (Kozmon, Stanislav); Tvaroska, I (Tvaroska, Igor); Koca, J (Koca, Jaroslav)
Source: GLYCOBIOLOGY **Volume:** 26 **Issue:** 7 **Pages:** 757-771 **DOI:** 10.1093/glycob/cww010 **Published:** JUL 2016
Abstract: The enzyme UDP-N-acetylglucosamine: alpha-D-mannoside beta-1-6 N-acetylglucosaminyltransferase V (GnT-V) catalyzes the transfer of GlcNAc from the UDP-GlcNAc donor to the alpha-1-6-linked mannose of the trimannosyl core structure of glycoproteins to produce the beta-1-6-linked branching of N-linked oligosaccharides. beta-1-6-GlcNAc-branched N-glycans are associated with cancer growth and metastasis. Therefore, the inhibition of GnT-V represents a key target for anti-cancer drug development. However, the development of potent and specific inhibitors of GnT-V is hampered by the lack of information on the three-dimensional structure of the enzyme and on the binding characteristics of its substrates. Here we present the first 3D structure of GnT-V as a result of homology modeling. Various alignment methods, docking the donor and acceptor substrates, and molecular dynamics simulation were used to construct seven homology models of GnT-V and characterize the binding of its substrates. The best homology model is consistent with available experimental data. The three-dimensional model, the structure of the enzyme catalytic site and binding information obtained for the donor and acceptor can be useful in studies of the catalytic mechanism and design of inhibitors of GnT-V.
Accession Number: WOS:000384766000009
PubMed ID: 26821880
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901

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Record 268 of 491
Title: Investigating the timing of origin and evolutionary processes shaping regional species diversity: Insights from simulated data and neotropical butterfly diversification rates
Author(s): Matos-Maravi, P (Matos-Maravi, Pavel)
Source: EVOLUTION **Volume:** 70 **Issue:** 7 **Pages:** 1638-1650 **DOI:** 10.1111/evo.12960 **Published:** JUL 2016
Abstract: Different diversification scenarios have been proposed to explain the origin of extant biodiversity. However, most existing meta-analyses of time-calibrated phylogenies rely on approaches that do not quantitatively test alternative diversification processes. Here, I highlight the shortcomings of using species divergence ranks, which is a method widely used in meta-analyses. Divergence ranks consist of categorizing cladogenetic events to certain periods of time, typically to either Pleistocene or to pre-Pleistocene ages. This approach has been claimed to shed light on the origin of most extant species and the timing and dynamics of diversification in any biogeographical region. However, interpretations drawn from such method often confound two fundamental questions in macroevolutionary studies, tempo (timing of evolutionary rate shifts) and mode ("how" and "why" of speciation). By using simulated phylogenies under four diversification scenarios, constant-rate, diversity-dependence, high extinction, and high speciation rates in the Pleistocene, I showed that interpretations based on species divergence ranks might have been seriously misleading. Future meta-analyses of dated phylogenies need to be aware of the impacts of incomplete taxonomic sampling, tree topology, and divergence time uncertainties, as well as they might be benefited by including quantitative tests of alternative diversification models that acknowledge extinction and diversity dependence.
Accession Number: WOS:000380023200017
PubMed ID: 27240554
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Matos-Maravi, Pavel	O-6626-2017	0000-0002-2885-4919

ISSN: 0014-3820
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Record 269 of 491
Title: Doping-induced stability in vanadium-doped ZnO quantum well wires (QWW): Combination of DFT calculations within experimental measurements
Author(s): Yumak, A (Yumak, A.); Goumri-Said, S (Goumri-Said, Souraya); Khan, W (Khan, Wilayat); Boubaker, K (Boubaker, Karem); Petkova, P (Petkova, P.)
Source: SOLID STATE SCIENCES **Volume:** 57 **Pages:** 33-37 **DOI:** 10.1016/j.solidstatesciences.2016.04.010 **Published:** JUL 2016

Abstract: ZnO quantum well wires (QWW) have grown on glass substrates by an inexpensive, simplified and enhanced spray pyrolysis technique then doped by Vanadium. The effects of V-doping on the structural, morphological and optical properties of the QWW were investigated experimentally and theoretically. The accuracy of control can be achieved on functional performance by adjusting vanadium doping extent. The incorporation of Vanadium in ZnO-QWW induced the formation of band tailing in states. The interactions with phonons and the presence of a tail absorption profile are following the empirical Urbach law. The electronic structure using density functional theory have shown the changes induced by vanadium doping in ZnO-QWW, where the phonon band structure and density of states were reported. The DFT results showed a good agreement with the lattice compatibility theory as well as with the experimental results. (C) 2016 Elsevier Masson SAS. All rights reserved.

Accession Number: WOS:000378960300005

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862

ISSN: 1293-2558
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Record 270 of 491

Title: Market mechanism design for profitable on-demand transport services

Author(s): Egan, M (Egan, Malcolm); Jakob, M (Jakob, Michal)

Source: TRANSPORTATION RESEARCH PART B-METHODOLOGICAL **Volume:** 89 **Pages:** 178-195 **DOI:** 10.1016/j.trb.2016.04.020 **Published:** JUL 2016

Abstract: On-demand transport services in the form of dial-a-ride and taxis are crucial parts of the transport infrastructure in all major cities. However, not all on-demand transport services are equal: not-for-profit dial-a-ride services with coordinated drivers significantly differ from profit-motivated taxi services with uncoordinated drivers. In fact, there are two key threads of work on efficient scheduling, routing, and pricing for passengers: dial-a-ride services; and taxi services. Unfortunately, there has been only limited development of algorithms for joint optimization of scheduling, routing, and pricing; largely due to the widespread assumption of fixed pricing. In this paper, we introduce another thread: profit motivated on-demand transport services with coordinated drivers. To maximize provider profits and the efficiency of the service, we propose a new market mechanism for this new thread of on-demand transport services, where passengers negotiate with the service provider. In contrast to previous work, our mechanism jointly optimizes scheduling, routing, and pricing. Ultimately, we demonstrate that our approach can lead to higher profits and reduced passenger prices, compared with standard fixed price approaches, while also improving efficiency. (C) 2016 Elsevier Ltd. All rights reserved.

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Record 271 of 491

Title: Functional analysis of the p.(Leu15Pro) and p.(Gly20Arg) sequence changes in the signal sequence of LDL receptor

Author(s): Pavlouskova, J (Pavlouskova, Jana); Reblova, K (Reblova, Kamila); Tichy, L (Tichy, Lukas); Freiberger, T (Freiberger, Tomas); Fajkusova, L (Fajkusova, Lenka)

Source: ATHEROSCLEROSIS **Volume:** 250 **Pages:** 9-14 **DOI:** 10.1016/j.atherosclerosis.2016.04.022 **Published:** JUL 2016

Abstract: The low density lipoprotein receptor (LDLR) is a transmembrane protein that plays a key role in cholesterol metabolism. It contains 860 amino acids including a 21 amino acid long signal sequence, which directs the protein into the endoplasmic reticulum. Mutations in the LDLR gene lead to cholesterol accumulation in the plasma and results in familial hypercholesterolemia (FH). Knowledge of the impact of a mutation on the LDLR protein structure and function is very important for the diagnosis and management of FH. Unfortunately, for a large proportion of mutations this information is still missing. In this study, we focused on the LDLR signal sequence and carried out functional and in silico analyses of two sequence changes, p.(Gly20Arg) and p.(Leu15Pro), localized in this part of the LDLR. Our results revealed that the p.(Gly20Arg) change, previously described as disease causing, has no detrimental effect on protein expression or LDL particle binding. In silico analysis supports this observation, showing that both the wt and p.(Gly20Arg) signal sequences adopt an expected alpha-helix structure. In contrast, the mutation p.(Leu15Pro) is not associated with functional protein expression and exhibits a structure with disrupted a alpha-helical arrangement in the signal sequence, which most likely affects protein folding in the endoplasmic reticulum. (C) 2016 Elsevier Ireland Ltd. All rights reserved.

Accession Number: WOS:000377982800002
PubMed ID: 27175606

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Freiberger, Tomas	D-8421-2011	0000-0001-6532-7053

ISSN: 0021-9150
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Record 272 of 491

Title: New version of hex-ecs, the B-spline implementation of exterior complex scaling method for solution of electron-hydrogen scattering

Author(s): Benda, J (Benda, Jakub); Houfek, K (Houfek, Karel)

Source: COMPUTER PHYSICS COMMUNICATIONS **Volume:** 204 **Pages:** 216-217 **DOI:** 10.1016/j.cpc.2016.03.020 **Published:** JUL 2016
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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houfek, Karel	P-2300-2017	0000-0002-7974-0399
Benda, Jakub		0000-0003-0965-2040

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Record 273 of 491

Title: Mammalian X homolog acts as sex chromosome in lacertid lizards

Author(s): Rovatsos, M (Rovatsos, M.); Vukic, J (Vukic, J.); Kratochvil, L (Kratochvil, L.)

Source: HEREDITY **Volume:** 117 **Issue:** 1 **Pages:** 8-13 **DOI:** 10.1038/hdy.2016.18 **Published:** JUL 2016

Abstract: Among amniotes, squamate reptiles are especially variable in their mechanisms of sex determination; however, based largely on cytogenetic data, some lineages possess highly evolutionary stable sex chromosomes. The still very limited knowledge of the genetic content of squamate sex chromosomes precludes a reliable reconstruction of the evolutionary history of sex determination in this group and consequently in all amniotes. Female heterogamety with a degenerated W chromosome typifies the lizards of the family Lacertidae, the widely distributed Old World clade including several hundreds of species. From the liver transcriptome of the lacertid Takydromus sexlineatus female, we selected candidates for Z-specific genes as the loci lacking single-nucleotide polymorphisms. We validated the candidate genes through the comparison of the copy numbers in the female and male genomes of T. sexlineatus and another lacertid species, Lacerta agilis, by quantitative PCR that also proved to be a reliable technique for the molecular sexing of the studied species. We suggest that this novel approach is effective for the detection of Z-specific and X-specific genes in lineages with degenerated W, respectively Y chromosomes. The analyzed gene content of the Z chromosome revealed that lacertid sex chromosomes are not homologous with those of other reptiles including birds, but instead the genes have orthologs in the X-conserved region shared by viviparous mammals. It is possible that this part of the vertebrate genome was independently co-opted for the function of sex chromosomes in viviparous mammals and lacertids because of its content of genes involved in gonad differentiation.

Accession Number: WOS:000377495900002
PubMed ID: 26980341

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kratochvil, Lukas	A-1997-2008	0000-0002-3515-729X
Rovatsos, Michail	D-3559-2013	0000-0002-8429-5680
Vukic, Jasna	D-2811-2015	0000-0003-2243-0303

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Record 274 of 491

Title: The electrostatic co-assembly in non-stoichiometric aqueous mixtures of copolymers composed of one neutral water-soluble and one polyelectrolyte (either positively or negatively charged) block: a dissipative particle dynamics study

Author(s): Sindelka, K (Sindelka, Karel); Limpouchova, Z (Limpouchova, Zuzana); Lisal, M (Lisal, Martin); Prochazka, K (Prochazka, Karel)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 24 **Pages:** 16137-16151 **DOI:** 10.1039/c6cp01047d **Published:** JUN 28 2016

Abstract: The electrostatic co-assembly in non-stoichiometric aqueous mixtures of diblock copolymers composed of a neutral water-soluble block and an either positively or negatively charged polyelectrolyte (PE) block has been studied by dissipative particle dynamics (DPD) simulations. The employed DPD variant includes explicit electrostatics and enables the investigation of the role of small ions in the co-assembly. The properties of core-shell associates containing insoluble interpolyelectrolyte complex cores and protective neutral shells were investigated as functions of the ratio of positive-to-negative charges in the system. This ratio was varied by increasing the number of positively charged PE chains of the same length as those of negatively charged chains, and by changing the PE length and charge density. The simulation results show that the associates formed in non-stoichiometric mixtures differ from those formed in stoichiometric mixtures: their association numbers are lower, their cores are charged and a fraction of excess chains remain free in the non-associated state. The study demonstrates the important role of the compatibility of the counterions with the polymer blocks. It simultaneously emphasizes the necessity of including the electrostatic interaction of all the charged species in the DPD computational scheme.

Accession Number: WOS:000381056500010

PubMed ID: 27253089

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Limpouchova, Zuzana	C-7791-2013	0000-0002-2290-1358
Sindelka, Karel	E-8790-2014	0000-0003-3925-924X
Lisal, Martin	A-8176-2011	0000-0001-8005-7143
Prochazka, Karel	C-3012-2014	0000-0003-2144-5378

ISSN: 1463-9076

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Record 275 of 491

Title: Interaction of Gold with a Pinwheel TiO similar to 1.2 Film Formed on Rh(111) Facet: STM and DFT Studies

Author(s): Mutombo, P (Mutombo, Pingo); Gubo, R (Gubo, Richard); Berko, A (Berko, Andras)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 120 **Issue:** 23 **Pages:** 12917-12923 **DOI:** 10.1021/acs.jpcc.6b03959 **Published:** JUN 16 2016

Abstract: The atomic structure of "pinwheel" TiO similar to 1.2 ultrathin oxide (w-TiO-UTO) layer and its reaction with gold are studied by scanning tunneling microscopy (STM) imaging, and density functional theory (DFT) calculations. The UTO film was formed as an encapsulation layer on the top facet (111) of stripe-like Rh nanoparticles supported on a TiO2(110) substrate. For proposing a structural model, the previous STM, photoelectron (XPS), and ion scattering spectroscopy (LEIS) results were also taken into account. DFT calculations were carried out within the generalized gradient approximation (GGA-PBE) in the frame of the Quantum Espresso code. A Rh(111) slab of four layers with a TiO1.14 overlayer and a Rh-Ti-O stacking sequence were used. In the starting model, the ratio between hcp and fcc sites filled With Ti atoms was 1.54 (the same value for O atoms was 2.2) on the top of Rh layers. The simulation of the STM images of the relaxed structure was done following the Tersoff-Hamann approximation. The main structural characteristics obtained experimentally were successfully reproduced in the simulation results: (i) the chemical contrast appeared as a pinwheel structure and (ii) compared with an ideal hexagonal lattice, characteristic local distortions were found in the UTO film. In harmony with the experimental results, the DFT calculations of the adsorption of a single Au atom on a w-TiO-UTO layer indicated that there is a characteristic site preference within the unit cell of the UTO film. This feature was also experimentally demonstrated for the early stage of the deposition of Au at room temperature, suggesting a moderate template effect adjusted by the pinwheel structure. This work demonstrates clearly that the lack of the so-called "nanoholes" does not completely cancel the template effect because the periodic lattice strain in itself substitutes their role. Moreover, the weaker modulation of Au/TiO-UTO bond permits the formation of one atomic layer thick 2D gold nanoparticles at 300 K.

Accession Number: WOS:000378196200062

Author Identifiers:

Author	ResearcherID Number	ORCID Number
COST, CM1104	I-8057-2015	
Gubo, Richard	C-4809-2018	0000-0001-6612-7264

ISSN: 1932-7447

Record 276 of 491

Title: Evanescent field optimization on Y-branch silicon nitride optical waveguide for biosensing

Author(s): Reshak, AH (Reshak, A. H.); Shahimin, MM (Shahimin, M. M.); Khor, KN (Khor, K. N.); Wahid, MHA (Wahid, M. H. A.); Hambali, NAMA (Hambali, N. A. M. Ahmad)

Source: MATERIALS LETTERS **Volume:** 173 **Pages:** 127-130 **DOI:** 10.1016/j.matlet.2016.02.142 **Published:** JUN 15 2016

Abstract: Evanescent field had been widely used in bio and chemical sensors. However in most cases, evanescent field is not maximized and consequently produced an unoptimized sensor performance. It is the aim of the paper to optimize the design of 1:2 Y-branch splitter optical waveguide through simulation by using FD-BPM. Y-branch splitter are simulated to optimize the power loss. Width of waveguide and effective angle are manipulated in the power loss optimization. The result shows that evanescent field is maximized at optimized thickness and width. The result suggests that Y-branch splitter with width of 25 um and effective angle of 6.24 is the best design for evanescent field sensor application with both high sensitivity and signal to noise ratio. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000374325900032

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363
Mohamad Shahimin, Mukhzeer	I-7646-2016	0000-0001-8644-5083

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Record 277 of 491

Title: Electronic and transport properties of the Mn-doped topological insulator Bi2Te3: A first-principles study

Author(s): Carva, K (Carva, K.); Kudrnovsky, J (Kudrnovsky, J.); Maca, F (Maca, F.); Drchal, V (Drchal, V.); Turek, I (Turek, I.); Balaz, P (Balaz, P.); Tkac, V (Tkac, V.); Holy, V (Holy, V.); Sechovsky, V (Sechovsky, V.); Honolka, J (Honolka, J.)

Source: PHYSICAL REVIEW B **Volume:** 93 **Issue:** 21 **Article Number:** 214409 **DOI:** 10.1103/PhysRevB.93.214409 **Published:** JUN 8 2016

Abstract: We present a first-principles study of the electronic, magnetic, and transport properties of the topological insulator Bi2Te3 doped with Mn atoms in substitutional (Mn-Bi) and interstitial van der Waals gap positions (Mn-i), which act as acceptors and donors, respectively. The effect of native Bi-Te- and Te-Bi-antisite defects and their influence on calculated electronic transport properties is also investigated. We have studied four models representing typical cases, namely, (i) Bi2Te3 with and without native defects, (ii) Mn-Bi defects with and without native defects, (iii) the same, but for Mn-i defects, and (iv) the combined presence of Mn-Bi and Mn-i. It has been found that lattice relaxations around Mn-Bi defects play an important role for both magnetic and transport properties. The resistivity is strongly influenced by the amount of carriers, their type, and by the relative positions of the Mn-impurity energy levels and the Fermi energy. Our results suggest strategies to tune bulk resistivities and also clarify the location of Mn atoms in samples. Calculations indicate that at least two of the considered defects have to be present simultaneously in order to explain the experimental observations, and the role of interstitials may be more important than expected.

Accession Number: WOS:000377299100003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Holy, Vaclav	E-1508-2017	0000-0002-0370-6928
Balaz, Pavel	M-9510-2015	0000-0003-0016-9271
Carva, Karel	A-3703-2008	0000-0002-2275-1986
Maca, Frantisek	G-4467-2014	
Sechovsky, Vladimir		0000-0003-1298-2120

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Record 278 of 491

Title: Nonlinear elastic effects in phase field crystal and amplitude equations: Comparison to ab initio simulations of bcc metals and graphene

Author(s): Huter, C (Hueter, Claas); Friak, M (Friak, Martin); Weikamp, M (Weikamp, Marc); Neugebauer, J (Neugebauer, Joerg); Goldenfeld, N (Goldenfeld, Nigel); Svendsen, B (Svendsen, Bob); Spatschek, R (Spatschek, Robert)

Source: PHYSICAL REVIEW B **Volume:** 93 **Issue:** 21 **Article Number:** 214105 **DOI:** 10.1103/PhysRevB.93.214105 **Published:** JUN 8 2016

Abstract: We investigate nonlinear elastic deformations in the phase field crystal model and derived amplitude equation formulations. Two sources of nonlinearity are found, one of them is based on geometric nonlinearity expressed through a finite strain tensor. This strain tensor is based on the inverse right Cauchy-Green deformation tensor and correctly describes the strain dependence of the stiffness for anisotropic and isotropic behavior. In isotropic one-and two-dimensional situations, the elastic energy can be expressed equivalently through the left deformation tensor. The predicted isotropic low-temperature nonlinear elastic effects are directly related to the Birch-Murnaghan equation of state with bulk modulus derivative K' = 4 for bcc. A two-dimensional generalization suggests K'(2D) = 5. These predictions are in agreement with ab initio results for large strain bulk deformations of various bcc elements and graphene. Physical nonlinearity arises if the strain dependence of the density wave amplitudes is taken into account and leads to elastic weakening. For anisotropic deformation, the magnitudes of the amplitudes depend on their relative orientation to the applied strain.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Svendsen, Bob	D-6311-2014	0000-0002-1519-9433

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Record 279 of 491

Title: Advanced SPARQL querying in small molecule databases

Author(s): Galgonek, J (Galgonek, Jakub); Hurt, T (Hurt, Tomas); Michlikova, V (Michlikova, Vendula); Onderka, P (Onderka, Petr); Schwarz, J (Schwarz, Jan); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF CHEMINFORMATICS **Volume:** 8 **Article Number:** 31 **DOI:** 10.1186/s13321-016-0144-4 **Published:** JUN 6 2016

Abstract: Background: In recent years, the Resource Description Framework (RDF) and the SPARQL query language have become more widely used in the area of cheminformatics and bioinformatics databases. These technologies allow better interoperability of various data sources and powerful searching facilities. However, we identified several deficiencies that make usage of such RDF databases restrictive or challenging for common users.
Results: We extended a SPARQL engine to be able to use special procedures inside SPARQL queries. This allows the user to work with data that cannot be simply precomputed and thus cannot be directly stored in the database. We designed an algorithm that checks a query against data ontology to identify possible user errors. This greatly improves query debugging. We also introduced an approach to visualize retrieved data in a user-friendly way, based on templates describing visualizations of resource classes. To integrate all of our approaches, we developed a simple web application.
Conclusions: Our system was implemented successfully, and we demonstrated its usability on the ChEBI database transformed into RDF form. To demonstrate procedure call functions, we employed compound similarity searching based on OrChem. The application is publicly available at https://bioinfo.uochb.cas.cz/projects/chemRDF.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Galgonek, Jakub		0000-0002-7038-544X

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Record 280 of 491

Title: DFT study of zigzag (n, 0) single-walled carbon nanotubes: C-13 NMR chemical shifts

Author(s): Kupka, T (Kupka, Teobald); Stachow, M (Stachow, Michal); Stobinski, L (Stobinski, Leszek); Kaminsky, J (Kaminsky, Jakub)

Source: JOURNAL OF MOLECULAR GRAPHICS & MODELLING **Volume:** 67 **Pages:** 14-19 **DOI:** 10.1016/j.jmgm.2016.04.008 **Published:** JUN 2016

Abstract: C-13 NMR chemical shifts of selected finite-size models of pristine zigzag single walled carbon nanotubes (SWCNTs) with a diameter of similar to 0.4-0.8 nm and length up to 2.2 nm were studied theoretically. Results for finite SWCNTs models containing 1, 4 and 10 adjacent bamboo-type units were compared with data obtained for infinite tubes in order to estimate the reliability of small finite models in predicting magnetic properties of real-size nanotubes and to assess their tube-length dependence. SWCNTs were fully optimized using unrestricted density functional theory (DFT-UB3LYP/6-31G*). Cyclacenes, as the shortest models of open-ended zigzag SWCNTs, with systematically varying diameter were calculated as well. GIAO NMR calculations on the SWCNT and cyclacene models were performed using the BH and H density functional combined with relatively small STO-3G(mag) basis set, developed by Leszczyriski and coworkers for accurate description of magnetic properties. Regular changes of carbon C-13 chemical shifts along the tube axis of real size (6, 0) and (9, 0) zigzag carbon nanotubes were shown. The C-13 NMR shifts according to increasing diameter calculated for zigzag (n, 0, n=5-10) cyclacenes followed the trends observed for zigzag (n, 0) SWCNTs. The results for 4-units long SWCNTs match reasonably well with the data obtained for infinite zigzag (n, 0) SWCNTs, especially to those with bigger diameter (n = 8-15). The presence of rim hydrogens obviously affects theoretical C-13 chemical shieldings and shifts in cyclacenes and thus cyclacenes can provide only approximate estimation of C-13 NMR parameters of real-size SWCNTs. The NMR properties predicted for the longest 10-units long models of SWCNTs reliably correspond to results obtained for infinite nanotubes. They were thus able to accurately predict also recently reported experimental chemical shift of chiral (6, 5) SWCNT.

Accession Number: WOS:000379632200002

PubMed ID: 27155813

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022
Kupka, Teobald		0000-0002-6252-3822

ISSN: 1093-3263
eISSN: 1873-4243

Record 281 of 491

Title: Evolutionary relationships within the Phytophthora cactorum species complex in Europe

Author(s): Panek, M (Panek, Motej); Fer, T (Fer, Tomas); Mracek, J (Mracek, Joroslav); Tomsovsky, M (Tomsovsky, Michal)

Source: FUNGAL BIOLOGY **Volume:** 120 **Issue:** 6-7 **Pages:** 836-851 **DOI:** 10.1016/j.funbio.2016.03.006 **Published:** JUN-JUL 2016

Abstract: The Phytophthora cactorum species complex in Europe is composed of P. cactorum, Phytophthora hedraiandra, and a hybrid species Phytophthora x serendipita. Evolutionary analyses using the amplified fragment length polymorphism (APLP) method were carried out on 133 isolates from 19 countries. The AFLP data were complemented by sequence analysis of three genes (ITS region of ribosomal RNA gene, phenolic acid decarboxylase - Pheca I, and Cytochrome oxidase Cox I), morphometric analysis and cardinal temperature data. The high proportion of clonal genotypes, low gene flow among groups, which was defined by the structure analysis, and low Nei's gene diversity confirms the

homothallic life cycle of the groups. On the other hand, the ITS, Cox I and Pheca I sequence data support occasional hybridization between species. The structure K = 5 grouping revealed two groups of hybrid origin (C2 and F). While the C2 group resembles P. x serendipita, the F group includes Finnish isolates characterized by high oogonial abortion rates and slow growth. The morphological characters routinely used in identification of Phytophthora species are not useful for delimitation of species from the P. cactorum complex. Therefore, we discuss the status of P. hedraiandra as a separate species. The epitypification of P. cactorum is proposed. (C) 2016 British Mycological Society. Published by Elsevier Ltd. All rights reserved.

Accession Number: WOS:000378665800003

PubMed ID: 27268244

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Tomsovsky, Michal	B-1263-2014	0000-0002-9505-6175
Fer, Tomas	A-9991-2008	0000-0002-0126-3684

ISSN: 1878-6146

eISSN: 1878-6162

Record 282 of 491

Title: Rayleigh scattering in the atmospheres of hot stars

Author(s): Fisak, J (Fisak, J.); Krticka, J (Krticka, J.); Munzar, D (Munzar, D.); Kubat, J (Kubat, J.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 590 **Article Number:** A95 **DOI:** 10.1051/0004-6361/201628291 **Published:** JUN 2016

Abstract: Context. Rayleigh scattering is a result of an interaction of photons with bound electrons. Rayleigh scattering is mostly neglected in calculations of hot star model atmospheres because most of the hydrogen atoms are ionized and the heavier elements have a lower abundance than hydrogen. In atmospheres of some chemically peculiar stars, helium overabundant regions containing singly ionized helium are present and Rayleigh scattering can be a significant opacity source.
Aims. We evaluate the contribution of Rayleigh scattering by neutral hydrogen and singly ionized helium in the atmospheres of hot stars with solar composition and in the atmospheres of helium overabundant stars.
Methods. We computed several series of model atmospheres using the TLUSTY code and emergent fluxes using the SYNSPEC code. These models describe atmospheres of main sequence B-type stars with different helium abundance. We used an existing grid of models for atmospheres with solar chemical composition and we calculated an additional grid for helium-rich stars with N(He)/N(H) = 10.
Results. Rayleigh scattering by neutral hydrogen can be neglected in atmospheres of hot stars, while Rayleigh scattering by singly ionized helium can be a non-negligible opacity source in some hot stars, especially in helium-rich stars.

Accession Number: WOS:000378106800118

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kubat, Jiri	G-9032-2014	0000-0003-4269-8278

ISSN: 1432-0746

Record 283 of 491

Title: Cytauxzoon Infections in Wild Felids from Carpathian-Danubian-Pontic Space: Further Evidence for a Different Cytauxzoon Species in European Felids

Author(s): Gallusova, M (Gallusova, Martina); Jirsova, D (Jirsova, Dagmar); Mihalca, AD (Mihalca, Andrei D.); Gherman, CM (Gherman, Calin Mircea); D'Amico, G (D'Amico, Gianluca); Qablan, MA (Qablan, Moneeb A.); Modry, D (Modry, David)

Source: JOURNAL OF PARASITOLOGY **Volume:** 102 **Issue:** 3 **Pages:** 377-380 **DOI:** 10.1645/15-881 **Published:** JUN 2016

Abstract: Parasitic protists of the genus Cytauxzoon are detected in a wide range of wild and domestic felids. Bobcats are a confirmed reservoir of Cytauxzoon felis in North America while domestic cats are susceptible hosts suffering from severe or fatal illness. Cytauxzoon infections are mainly reported from American felids and, recently, several sub-clinical and clinical findings were reported from European, Asian, and African felids. In 2014, the collection of organs of 4 Eurasian lynx and 12 wild cats from 11 Romanian localities was carried out to determine the prevalence and genetic diversity of Cytauxzoon spp. We detected an overall high prevalence of 62.5% in both species of wild felids; 50% in wild cats and 100% in Eurasian lynx. The phylogenetic analysis indicates 2 distinct clades of Cytauxzoon in felids, with all of our sequences clustering with sequences of Cytauxzoon sp./Cytauxzoon manul from Palaearctic felids. Further studies, development of new genetic markers, and experimental transmission studies are required for clarifying the taxonomy and life cycle of feline Cytauxzoon in the Old World.

Accession Number: WOS:000378093400011

PubMed ID: 26741977

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mihalca, Andrei	A-1561-2008	0000-0001-6076-7914
gherman, calin	P-5823-2016	0000-0002-5936-2538
Modry, David	G-7815-2014	

ISSN: 0022-3395

eISSN: 1937-2345

Record 284 of 491

Title: Spectroscopic properties of the triple bond carotenoid alloxanthin

Author(s): West, R (West, Robert); Kesan, G (Kesan, Gurkan); Trskova, E (Trskova, Eliska); Sobotka, R (Sobotka, Roman); Kana, R (Kana, Radek); Fuciman, M (Fuciman, Marcel); Polivka, T (Polivka, Tomas)

Source: CHEMICAL PHYSICS LETTERS **Volume:** 653 **Pages:** 167-172 **DOI:** 10.1016/j.cplett.2016.04.085 **Published:** JUN 1 2016

Abstract: Alloxanthin, which has two triple bonds within its backbone, was studied by steady-state and femtosecond transient absorption spectroscopies. Alloxanthin demonstrates an S-2 energy comparable to its non-triple bond homolog, zeaxanthin, while the S-1 lifetime of 19 ps is markedly longer than that of zeaxanthin (9 ps). Along with corroborating quantum chemistry calculations, the results show that the long-lived S1 state of alloxanthin, which typically corresponds to the dynamic of a shorter carotenoid backbone, implies the triple bond isolates the conjugation of the backbone, increasing the S-1 state energy and diminishing the S-1-S-2 energy gap. (C) 2016 Elsevier B.V. All rights reserved.

Accession Number: WOS:000377206400029

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kana, Radek	A-6434-2009	0000-0001-5768-6902
Sobotka, Roman	J-3077-2014	0000-0001-5909-3879
Polivka, Tomas	G-9564-2014	0000-0002-6176-0420

ISSN: 0009-2614

eISSN: 1873-4448

Record 285 of 491

Title: The impact of new Geant4-DNA cross section models on electron track structure simulations in liquid water

Author(s): Kyriakou, I (Kyriakou, I.); Sefl, M (Sefl, M.); Nourry, V (Nourry, V.); Incerti, S (Incerti, S.)

Source: JOURNAL OF APPLIED PHYSICS **Volume:** 119 **Issue:** 19 **Article Number:** 194902 **DOI:** 10.1063/1.4950808 **Published:** MAY 21 2016

Abstract: The most recent release of the open source and general purpose Geant4 Monte Carlo simulation toolkit (Geant4 10.2 release) contains a new set of physics models in the Geant4-DNA extension for improving the modelling of low-energy electron transport in liquid water (<10 keV). This includes updated electron cross sections for excitation, ionization, and elastic scattering. In the present work, the impact of these developments to track-structure calculations is examined for providing the first comprehensive comparison against the default physics models of Geant4-DNA. Significant differences with the default models are found for the average path length and penetration distance, as well as for dose-point-kernels for electron energies below a few hundred eV. On the other hand, self-irradiation absorbed fractions for tissue-like volumes and low-energy electron sources (including

some Auger emitters) reveal rather small differences (up to 15%) between these new and default Geant4-DNA models. The above findings indicate that the impact of the new developments will mainly affect those applications where the spatial pattern of interactions and energy deposition of very-low energy electrons play an important role such as, for example, the modelling of the chemical and biophysical stage of radiation damage to cells. Published by AIP Publishing.

Accession Number: WOS:000377718100026

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Incerti, Sebastien	T-3006-2017	0000-0002-0619-2053
Sefl, Martin		0000-0003-2164-6620

ISSN: 0021-8979

eISSN: 1089-7550

Record 286 of 491

Title: Chemisorption of Acetophenone on Si(111)-7 x 7. Polar Aromatic Molecule on Electronically Complex Surface

Author(s): Krejci, O (Krejci, O.); Matvija, P (Matvija, P.); Zimmermann, P (Zimmermann, P.); Sobotik, P (Sobotik, P.); Ost'adal, I (Ost'adal, Ivan); Kocan, P (Kocan, P.)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 120 **Issue:** 17 **Pages:** 9200-9206 **DOI:** 10.1021/acs.jpcc.6b00486 **Published:** MAY 5 2016

Abstract: Temperature-dependent chemisorption of acetophenone molecules on the Si(111)-7 X 7 reconstruction was studied by means of scanning tunneling microscopy, scanning tunneling spectroscopy, and density functional theory calculations. A configuration interpreted as a silyl enolether has been repeatedly observed on the surface at room temperature and after annealing to 75 degrees C. The most frequent structure on the surface stable up to 150 degrees C is identified as a 1,6-adduct to two adatoms of the neighboring half unit cells. The results suggest that presence of the polar group in the molecule affects the chemisorption in a way that leads to bonding with two adatoms.

Accession Number: WOS:000375631100022

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kocan, Pavel	A-5060-2008	0000-0002-7677-557X
Zimmermann, Petr	O-7885-2017	0000-0001-7101-0378
Krejci, Ondrej	G-5918-2014	0000-0002-4948-4312
Sobotik, Pavel	O-9514-2017	0000-0002-8133-7742
Ostadal, Ivan	A-6870-2008	0000-0002-3458-7837
Matvija, Peter	O-5761-2017	0000-0002-1567-6930

ISSN: 1932-7447

Record 287 of 491

Title: Unification of ground-state aromaticity criteria - structure, electron delocalization, and energy - in light of the quantum chemical topology

Author(s): Badri, Z (Badri, Zahra); Foroutan-Nejad, C (Foroutan-Nejad, Cina)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 17 **Pages:** 11693-11699 **DOI:** 10.1039/c5cp05222j **Published:** MAY 2 2016

Abstract: In the present account we investigate a theoretical link between the bond length, electron sharing, and bond energy within the context of quantum chemical topology theories. The aromatic stabilization energy, ASE, was estimated from this theoretical link without using isodesmic reactions for the first time. The ASE values obtained from our method show a meaningful correlation with the number of electrons contributing to the aromaticity. This theoretical link demonstrates that structural, electronic, and energetic criteria of aromaticity - ground-state aromaticity - belong to the same class and guarantees that they assess the same property as aromaticity. Theory suggests that interatomic exchange-correlation potential, obtained from the theory of Interacting Quantum Atoms (IQA), is linearly connected to the delocalization index of Quantum Theory of Atoms in Molecules (QTAIM) and the bond length through a first order approximation. Our study shows that the relationship between energy, structure and electron sharing marginally deviates from the ideal linear form expected from the first order approximation. The observed deviation from linearity was attributed to a different contribution of exchange-correlation to the bond energy for the sigma- and pi-frameworks. Finally, we proposed two-dimensional energy-structure-based aromaticity indices in analogy to the electron sharing indices of aromaticity.

Accession Number: WOS:000375623100014

PubMed ID: 26678719

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173

ISSN: 1463-9076

eISSN: 1463-9084

Record 288 of 491

Title: CAVER: Algorithms for Analyzing Dynamics of Tunnels in Macromolecules

Author(s): Pavelka, A (Pavelka, Antonin); Sebestova, E (Sebestova, Eva); Kozlikova, B (Kozlikova, Barbora); Brezovsky, J (Brezovsky, Jan); Sochor, J (Sochor, Jiri); Damborsky, J (Damborsky, Jiri)

Source: IEEE-ACM TRANSACTIONS ON COMPUTATIONAL BIOLOGY AND BIOINFORMATICS **Volume:** 13 **Issue:** 3 **Pages:** 505-517 **DOI:** 10.1109/TCBB.2015.2459680 **Published:** MAY-JUN 2016

Abstract: The biological function of a macromolecule often requires that a small molecule or ion is transported through its structure. The transport pathway often leads through void spaces in the structure. The properties of transport pathways change significantly in time; therefore, the analysis of a trajectory from molecular dynamics rather than of a single static structure is needed for understanding the function of pathways. The identification and analysis of transport pathways are challenging because of the high complexity and diversity of macromolecular shapes, the thermal motion of their atoms, and the large amount of conformations needed to properly describe conformational space of protein structure. In this paper, we describe the principles of the CAVER 3.0 algorithms for the identification and analysis of properties of transport pathways both in static and dynamic structures. Moreover, we introduce the improved clustering solution for finding tunnels in macromolecules, which is included in the latest CAVER 3.02 version. Voronoi diagrams are used to identify potential pathways in each snapshot of a molecular dynamics trajectory and clustering is then used to find the correspondence between tunnels from different snapshots. Furthermore, the geometrical properties of pathways and their evolution in time are computed and visualized.

Accession Number: WOS:000378528100010

PubMed ID: 27295634

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Brezovsky, Jan	C-8290-2012	0000-0001-9677-5078
Kozlikova, Barbora	G-3890-2014	
Damborsky, Jiri	H-3799-2012	0000-0002-7848-8216

ISSN: 1545-5963

eISSN: 1557-9964

Record 289 of 491

Title: Transmembrane Potential Modeling: Comparison between Methods of Constant Electric Field and Ion Imbalance

Author(s): Melcr, J (Melcr, Josef); Bonhenry, D (Bonhenry, Daniel); Timr, S (Timr, Stepan); Jungwirth, P (Jungwirth, Pavel)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 12 **Issue:** 5 **Pages:** 2418-2425 **DOI:** 10.1021/acs.jctc.5b01202 **Published:** MAY 2016

Abstract: Two approaches for modeling of the transmembrane potential, as present in all eukaryotic cells, are examined in detail and compared with each other. One approach-uses an externally applied electric field, whereas the other maintains an imbalance of ions on the two sides of a membrane. We demonstrate that both methods provide converged results concerning structural parameters of the membrane which are practically indistinguishable from each other, at least for monovalent ions. Effects of the electric field on the detailed molecular structure of the phospholipid bilayer are also presented and discussed. In addition, we achieve a considerable speed-up of the underlying molecular dynamics simulations by implementing the virtual interaction sites method for the Slipids force field.

Accession Number: WOS:000375810000028
PubMed ID: 27014925
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bonhenry, Daniel	K-6336-2017	
Timr, Stepan	G-5313-2014	0000-0002-5824-4476
Jungwirth, Pavel	D-9290-2011	0000-0002-6892-3288

ISSN: 1549-9618
eISSN: 1549-9626

Record 290 of 491
Title: Circular Dichroism is Sensitive to Monovalent Cation Binding in Monensin Complexes
Author(s): Nedzhib, A (Nedzhib, Ahmed); Kessler, J (Kessler, Jiri); Bour, P (Bour, Petr); Gyurcsik, B (Gyurcsik, Bela); Pantcheva, I (Pantcheva, Ivayla)
Source: CHIRALITY **Volume:** 28 **Issue:** 5 **Pages:** 420-428 **DOI:** 10.1002/chir.22597 **Published:** MAY 2016
Abstract: Monensin is a natural antibiotic that exhibits high affinity to certain metal ions. In order to explore its potential in coordination chemistry, circular dichroism (CD) spectra of monensic acid A (MonH) and its derivatives containing monovalent cations (Li+, Na+, K+, Rb+, Ag+, and Et4N+) in methanolic solutions were measured and compared to computational models. Whereas the conventional CD spectroscopy allowed recording of the transitions down to 192nm, synchrotron radiation circular dichroism (SRCD) revealed other bands in the 178-192nm wavelength range. CD signs and intensities significantly varied in the studied compounds, in spite of their similar crystal structure. Computational modeling based on the Density Functional Theory (DFT) and continuum solvent model suggests that the solid state monensin structure is largely conserved in the solutions as well. Time-dependent Density Functional Theory (TDDFT) simulations did not allow band-to-band comparison with experimental spectra due to their limited precision, but indicated that the spectral changes were caused by a combination of minor conformational changes upon the monovalent cation binding and a direct involvement of the metal electrons in monensin electronic transitions. Both the experiment and simulations thus show that the CD spectra of monensin complexes are very sensitive to the captured ions and can be used for their discrimination. (C) 2016 Wiley Periodicals, Inc.
Accession Number: WOS:000375148300011
PubMed ID: 27062535
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kessler, Jiri	G-2880-2012	0000-0001-6307-4339
Gyurcsik, Bela	C-1851-2018	0000-0003-1894-7414

ISSN: 0899-0042
eISSN: 1520-636X

Record 291 of 491
Title: HMOG: New Behavioral Biometric Features for Continuous Authentication of Smartphone Users
Author(s): Sitova, Z (Sitova, Zdenka); Sedenka, J (Sedenka, Jaroslav); Yang, Q (Yang, Qing); Peng, G (Peng, Ge); Zhou, G (Zhou, Gang); Gasti, P (Gasti, Paolo); Balagani, KS (Balagani, Kiran S.)
Source: IEEE TRANSACTIONS ON INFORMATION FORENSICS AND SECURITY **Volume:** 11 **Issue:** 5 **Pages:** 877-892 **DOI:** 10.1109/TIFS.2015.2506542 **Published:** MAY 2016
Abstract: We introduce hand movement, orientation, and grasp (HMOG), a set of behavioral features to continuously authenticate smartphone users. HMOG features unobtrusively capture subtle micro-movement and orientation dynamics resulting from how a user grasps, holds, and taps on the smartphone. We evaluated authentication and biometric key generation (BKG) performance of HMOG features on data collected from 100 subjects typing on a virtual keyboard. Data were collected under two conditions: 1) sitting and 2) walking. We achieved authentication equal error rates (EERs) as low as 7.16% (walking) and 10.05% (sitting) when we combined HMOG, tap, and keystroke features. We performed experiments to investigate why HMOG features perform well during walking. Our results suggest that this is due to the ability of HMOG features to capture distinctive body movements caused by walking, in addition to the hand-movement dynamics from taps. With BKG, we achieved the EERs of 15.1% using HMOG combined with taps. In comparison, BKG using tap, key hold, and swipe features had EERs between 25.7% and 34.2%. We also analyzed the energy consumption of HMOG feature extraction and computation. Our analysis shows that HMOG features extracted at a 16-Hz sensor sampling rate incurred a minor overhead of 7.9% without sacrificing authentication accuracy. Two points distinguish our work from current literature: 1) we present the results of a comprehensive evaluation of three types of features (HMOG, keystroke, and tap) and their combinations under the same experimental conditions and 2) we analyze the features from three perspectives (authentication, BKG, and energy consumption on smartphones).
Accession Number: WOS:000372355200001
ISSN: 1556-6013
eISSN: 1556-6021

Record 292 of 491
Title: Magnetism and deformation of epitaxial Pd and Rh thin films
Author(s): Kana, T (Kana, Tomas); Huger, E (Huger, Erwin); Legut, D (Legut, Dominik); Cak, M (Cak, Miroslav); Sob, M (Sob, Mojmir)
Source: PHYSICAL REVIEW B **Volume:** 93 **Issue:** 13 **Article Number:** 134422 **DOI:** 10.1103/PhysRevB.93.134422 **Published:** APR 19 2016
Abstract: By means of ab initio calculations, we investigated structural and magnetic properties of Pd and Rh thin films, determining their lattice parameters and epitaxial stresses when they are grown on various substrates, and provided a comparison with available experimental data. Further, we studied in detail the magnetic properties of Pd in the higher-energy hcp structure and of Rh in the higher-energy bcc structure. The results predict that the hcp(11 (2) over bar0) Pd films [grown by epitaxy on the Nb(001) substrate] should not be ferromagnetically ordered. Concerning the hcp Pd, we mainly investigated the influence of the hcp c/a ratio on the hcp film stability and on the ferromagnetic order. It turns out that the c/a ratio has to be below 1.622 to induce the ferromagnetic order in hcp Pd. We proposed a technological route for obtaining ferromagnetic hcp(11 (2) over bar0) Pd films and explained the experimentally observed ferromagnetism in twinned Pd nanoparticles induced by strain. We also found that bcc Rh is ferromagnetically ordered, but it cannot be stabilized in the form of thin films. Therefore, we investigated the dependence of ferromagnetic order in bct Rh on the tetragonal c/a ratio and compared our results with experiments performed on Rh/Fe(001) multilayers.
Accession Number: WOS:000374528700003
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Rygelova, Pavla	B-7703-2009	0000-0001-7665-3276

ISSN: 2469-9950
eISSN: 2469-9969

Record 293 of 491
Title: Self-consistent quasiparticle formulation of a multiphonon method and its application to the neutron-rich O-20 nucleus
Author(s): De Gregorio, G (De Gregorio, G.); Knapp, F (Knapp, F.); Lo Iudice, N (Lo Iudice, N.); Vesely, P (Vesely, P.)
Source: PHYSICAL REVIEW C **Volume:** 93 **Issue:** 4 **Article Number:** 044314 **DOI:** 10.1103/PhysRevC.93.044314 **Published:** APR 15 2016
Abstract: A Bogoliubov quasiparticle formulation of an equation-of-motion phonon method, suited for open-shell nuclei, is derived. Like its particle-hole version, it consists of deriving a set of equations of motions whose iterative solution generates an orthonormal basis of n-phonon states (n = 0,1,2,...), built of quasiparticle Tamm-Dancoff phonons, which simplifies the solution of the eigenvalue problem. The method is applied to the open-shell neutron-rich O-20 for illustrative purposes. A Hartree-Fock-Bogoliubov canonical basis, derived from an intrinsic two-body optimized chiral Hamiltonian, is used to derive and solve the eigenvalue equations in a space encompassing a truncated two-phonon basis. The spurious admixtures induced by the violation of the particle number and the center-of-mass motion are eliminated to a large extent by a Gram-Schmidt orthogonalization procedure. The calculation takes into account the Pauli principle, is self-consistent, and is parameter free except for the energy cutoff used to truncate the two-phonon basis, which induces an increasing depression of the ground state through its strong coupling to the quasiparticle vacuum. Such a cutoff is fixed so as to reproduce the first 1(-) level. The two-phonon states are shown to enhance the level density of the low-energy spectrum, consistently with the data, and to induce a fragmentation of the E1 strength which, while accounting for the very low E1 transitions, is not sufficient to reproduce the experimental cross section in the intermediate energy region. This and other discrepancies suggest the need of including the

three-phonon states. These are also expected to offset the action of the two phonons on the quasiparticle vacuum and, therefore, free the calculation from any parameter.
Accession Number: WOS:000374297900002
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290
De Gregorio, Giovanni		0000-0003-0253-915X

ISSN: 2469-9985
eISSN: 2469-9993

Record 294 of 491
Title: BCFT moduli space in level truncation
Author(s): Kudrna, M (Kudrna, Matej); Maccaferri, C (Maccaferri, Carlo)
Source: JOURNAL OF HIGH ENERGY PHYSICS **Issue:** 4 **Article Number:** 057 **DOI:** 10.1007/JHEP04(2016)057 **Published:** APR 11 2016
Abstract: We propose a new non-perturbative method to search for marginal deformations in level truncated open string field theory. Instead of studying the flatness of the effective potential for the marginal field (which is not expected to give a one-to-one parametrization of the BCFT moduli space), we identify a new non-universal branch of the tachyon potential which, from known analytic examples, is expected to parametrize the marginal flow in a much larger region of the BCFT moduli space. By a level 18 computation in Siegel gauge we find an increasingly flat effective potential in the non-universal sector, connected to the perturbative vacuum and we confirm that the coefficient of the marginal field (ASFT) has a maximum compatible with the value where the solutions stop existing in the standard Sen-Zwiebach approach. At the maximal reachable level the effective potential still deviates from flatness for large values of the tachyon, but the Ellwood invariants stay close to the correct BCFT values on the whole branch and the full periodic moduli space of the cosine deformation is covered.
Accession Number: WOS:000374045100002
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Maccaferri, Carlo		0000-0002-1149-4726

ISSN: 1029-8479

Record 295 of 491
Title: Interaction of Ruthenium(II) with Terminal Alkynes: Benchmarking DFT Methods with Spectroscopic Data
Author(s): Skriba, A (Skriba, Anton); Jasik, J (Jasik, Juraj); Andris, E (Andris, Erik); Roithova, J (Roithova, Jana)
Source: ORGANOMETALLICS **Volume:** 35 **Issue:** 7 **Pages:** 990-994 **DOI:** 10.1021/acs.organomet.6b00021 **Published:** APR 11 2016
Abstract: Helium tagging infrared photodissociation (IRPD) spectroscopy for the characterization of organometallic complexes is presented. The IRPD spectrum of the [RuCp(PPh3)(PhCCH)](+) complex reveals that more than 80% of the detected ions correspond to a structure with pi-coordinated phenylacetylene, and the rest are complexes with the alkyne probably isomerized to its vinylidene form. The detected C=C and C H stretches of the terminal alkyne reflect the degree of activation of the triple bond. They are used to benchmark the popular DFT functionals used in theoretical studies of ruthenium catalysis. It is shown that there are only small differences between the methods. GGA methods (e.g., BP86 or PBEPBE) and (hybrid) meta GGA functionals (e.g., M06) provide slightly better descriptions of this system than hybrid DFT methods such as B3LYP. A notable exception is M06-2X, which significantly underestimates the activation of the C=C bond by the coordination to the ruthenium complex.
Accession Number: WOS:000374077200011
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Skriba, Anton	I-6651-2016	
Andris, Erik	O-2513-2017	0000-0002-9336-0157
Jasik, Juraj	O-1057-2017	0000-0002-1177-2837

ISSN: 0276-7333
eISSN: 1520-6041

Record 296 of 491
Title: Pt center dot center dot center dot H Nonclassical Interaction in Water-Dissolved Pt(II) Complexes: Coaction of Electronic Effects with Solvent-Assisted Stabilization
Author(s): Kroutil, O (Kroutil, Ondrej); Predota, M (Predota, Milan); Chval, Z (Chval, Zdenek)
Source: INORGANIC CHEMISTRY **Volume:** 55 **Issue:** 7 **Pages:** 3252-3264 **DOI:** 10.1021/acs.inorgchem.5b02261 **Published:** APR 4 2016
Abstract: The structure of the hydration shell of cisplatin, cis[Pt(NH3)(2)Cl-2], and its aquated derivatives cis-[Pt(NH3)(2)Cl(H2O)](+), cis-[Pt(NH3)(2)OH(H2O)](+), and cis-[Pt(NH3)(2)(H2O)(2)](2+) were studied by a number of density functional molecular dynamics (DFT-MD) simulations (from 30 to 250 ps) in which Pt(II) complexes were immersed in a periodic box with 72 explicit water molecules. Furthermore, Pt(II) complex-water binding energy curves and full DFT optimizations of dusters derived from the lowest potential energy DFT-MD frames offered a deeper insight into the structure of the first hydration shell and electronic changes connected with the formation of a nonclassical Pt center dot center dot center dot H-O-H (Pt center dot center dot center dot Hw) hydrogen bond (inverse hydration). The probability of a Pt center dot center dot center dot Hw interaction decreases with increasing charge of the platinum complex due to disadvantageous electrostatics. The main stabilization comes from the charge transfer being followed by polarization and dispersion. Ligands form a framework for the network of H-bond interactions between the solvent molecules, which play an important role in the promotion/suppression of the formation of the Pt center dot center dot center dot Hw interactions. In the +2 charged diaqua complex the Pt center dot center dot center dot Hw interaction is still attractive but cannot compete with classical H bonds between solvent molecules. Thus, the formation of a Pt center dot center dot center dot Hw interaction is the result of a suitable solvent H-bonding network and the probability of its incidence decreases with increasing flexibility of the solvent.
Accession Number: WOS:000373550700010
PubMed ID: 26974182
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Chval, Zdenek	D-8964-2016	0000-0003-1922-8390
Predota, Milan	A-2256-2009	0000-0003-3902-0992

ISSN: 0020-1669
eISSN: 1520-510X

Record 297 of 491
Title: Stimulation of ipt overexpression as a tool to elucidate the role of cytokinins in high temperature responses of Arabidopsis thaliana
Author(s): Skalak, J (Skalak, Jan); Cerny, M (Cerny, Martin); Jedelsky, P (Jedelsky, Petr); Dobra, J (Dobra, Jana); Ge, E (Ge, Eva); Novak, J (Novak, Jan); Hronkova, M (Hronkova, Marie); Dobrev, P (Dobrev, Petre); Vankova, R (Vankova, Radomira); Brzobohaty, B (Brzobohaty, Bretislav)
Source: JOURNAL OF EXPERIMENTAL BOTANY **Volume:** 67 **Issue:** 9 **Pages:** 2861-2873 **DOI:** 10.1093/jxb/erw129 **Published:** APR 2016
Abstract: Cytokinins (CKs) are phytohormones regulating plant growth and development as well as response to the environment. In order to evaluate their function in heat stress (HS) responses, the effect of CK elevation was determined during three types of HS - targeted to shoots, targeted to roots and applied to the whole plant. The early (30min) and longer term (3h) responses were followed at the hormonal, transcriptomic and proteomic levels in Arabidopsis transformants with dexamethasone-inducible expression of the CK biosynthetic gene isopentenyltransferase (ipt) and the corresponding wild-type (Col-0). Combination of hormonal and phenotypic analyses showed transient up-regulation of the CK/abscisic acid ratio, which controls stomatal aperture, to be more pronounced in the transformant. HS responses of the root proteome and Rubisco-immunodepleted leaf proteome were followed using 2-D gel electrophoresis and MALDI-TOF/TOF. More than 100 HS-responsive proteins were detected, most of them being modulated by CK increase. Proteome and transcriptome analyses demonstrated that CKs have longer term positive effects on the stress-related proteins and transcripts, as well as on the photosynthesis-related ones. Transient accumulation of CKs and stimulation of their signal transduction in tissue(s) not exposed to HS indicate that they are involved in plant stress responses.
Accession Number: WOS:000376385800028
PubMed ID: 27049021

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Hronkova, Marie	H-1558-2014	
Novak, Jan	I-3635-2014	
Cerny, Martin	D-7226-2012	
Kolaja Dobra, Jana	I-4026-2017	0000-0001-9503-6142
Jedelsky, Petr	C-5879-2009	0000-0003-3813-2343
Vankova, Radomira	G-6808-2014	0000-0001-9101-8844
Cerny, Martin		0000-0002-0651-4219

ISSN: 0022-0957
eISSN: 1460-2431

Record 298 of 491
Title: Rapid acidolysis of benzyl group as a suitable approach for syntheses of peptides naturally produced by oxidative stress and containing 3-nitrotyrosine
Author(s): Niederhafner, P (Niederhafner, Petr); Safarik, M (Safarik, Martin); Brichtova, E (Brichtova, Eva); Sebestik, J (Sebestik, Jaroslav)
Source: AMINO ACIDS **Volume:** 48 **Issue:** 4 **Pages:** 1087-1098 **DOI:** 10.1007/s00726-015-2163-2 **Published:** APR 2016
Abstract: 3-Nitrotyrosine (Nit) belongs to products of oxidative stress and could probably influence conformation of neurodegenerative proteins. Syntheses of peptides require availability of suitable synthon for introduction of Nit residue. Common phenolic protection groups are more acid labile, when they are attached to Nit residue. We have found that Fmoc-Nit(Bn)-OH is a good building block for syntheses of Nit containing peptides by Fmoc/tBu strategy. Interestingly, the peptides containing multiple Nit residues can be available solely by use of Fmoc-Nit(Bn)-OH synthon. Bn is removed rapidly with ca 80 % trifluoroacetic acid in dark. The cleavage of Bn from Fmoc-Nit(Bn)-OH proceeds via pseudo-first order mechanism with activation barrier 32 kcal mol(-1) and rate k = 15.3 s(-1) at 20 A degrees C. This rate is more than 2,000,000 times faster than that for cleavage of benzyl from Tyr(Bn).
Accession Number: WOS:000372551100018
PubMed ID: 26767371
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sebestik, Jaroslav	C-9166-2012	0000-0002-0614-2064

ISSN: 0939-4451
eISSN: 1438-2199

Record 299 of 491
Title: Real-life curriculum-based timetabling with elective courses and course sections
Author(s): Muller, T (Mueller, Tomas); Rudova, H (Rudova, Hana)
Source: ANNALS OF OPERATIONS RESEARCH **Volume:** 239 **Issue:** 1 **Pages:** 153-170 **DOI:** 10.1007/s10479-014-1643-1 **Published:** APR 2016
Abstract: This paper presents an innovative approach to curriculum-based timetabling. To capture complex relations of real life curriculum-based timetabling problems, curricula are defined by a rich model that includes optional courses and course groups among which students are expected to take a subset of courses. In addition, courses may contain alternative course sections. A transformation between the proposed curriculum model and student course enrollments is formalized and a local search algorithm generating corresponding enrollments is introduced. While the proposed curriculum model is too complicated for existing curriculum-based solvers, the transformation enables curriculum-based timetabling in any existing enrollment-based course timetabling solver. The approach was implemented in a well established enrollment-based course timetabling system UniTime. The system has been successfully applied in practice at the Faculty of Education at Masaryk University for about 7,500 students and 260 curricula and at the Faculty of Sports Studies at Masaryk University for about 1,400 students and 25 curricula. Experimental results related with these problems are demonstrated for two semesters.
Accession Number: WOS:000373223800009
ISSN: 0254-5330
eISSN: 1572-9338

Record 300 of 491
Title: Thermodynamic Properties of Molecular Crystals Calculated within the Quasi-Harmonic Approximation
Author(s): Cervinka, C (Cervinka, Ctirad); Fulem, M (Fulem, Michal); Stoffel, RP (Stoffel, Ralf Peter); Dronskowski, R (Dronskowski, Richard)
Source: JOURNAL OF PHYSICAL CHEMISTRY A **Volume:** 120 **Issue:** 12 **Pages:** 2022-2034 **DOI:** 10.1021/acs.jpca.6b00401 **Published:** MAR 31 2016
Abstract: A computational study of the possibilities of contemporary theoretical chemistry as regards calculated thermodynamic properties for molecular crystals from first principles is presented. The study is performed for a testing set of 22 low-temperature crystalline phases whose properties such as densities of phonon states, isobaric heat capacities, and densities are computed as functions of temperature within the quasi-harmonic approximation. Electronic structure and lattice dynamics are treated by plane-wave based calculations with optPBE-vdW functional. Comparison of calculated results with reliable critically assessed experimental data is especially emphasized.
Accession Number: WOS:000373416600010
PubMed ID: 26959684
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fulem, Michal	B-7450-2008	0000-0002-5707-0670
Cervinka, Ctirad	L-8310-2017	0000-0003-1498-6715

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Close

Web of Science
Page 7 (Records 301 -- 350)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

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Record 301 of 491

Title: Tip-induced gating of molecular levels in carbene-based junctions

Author(s): Foti, G (Foti, Giuseppe); Vazquez, H (Vazquez, Hector)

Source: NANOTECHNOLOGY **Volume:** 27 **Issue:** 12 **Article Number:** 125702 **DOI:** 10.1088/0957-4484/27/12/125702 **Published:** MAR 29 2016

Abstract: We study the conductance of N-heterocyclic carbene-based (NHC) molecules on gold by means of first-principles calculations based on density-functional theory and non-equilibrium Green's functions. We consider several tip structures and find a strong dependence of the position of the NHC molecular levels with the atomistic structure of the tip. The position of the lowest unoccupied molecular orbital (LUMO) can change by almost 0.8 eV with tip shape. Through an analysis of the net charge transfer, electron redistribution and work function for each tip structure, we rationalize the LUMO shifts in terms of the sum of the work function and the maximum electrostatic potential arising from charge rearrangement. These differences in the LUMO position, effectively gating the molecular levels, result in large conductance variations. These findings open the way to modulating the conductance of NHC-based molecular circuits through the controlled design of the tip atomistic structure.

Accession Number: WOS:000370442900020

PubMed ID: 26891059

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922

ISSN: 0957-4484

eISSN: 1361-6528

Record 302 of 491

Title: Structural and Electronic Properties of Nitrogen-Doped Graphene

Author(s): Sforzini, J (Sforzini, J.); Hapala, P (Hapala, P.); Franke, M (Franke, M.); van Straaten, G (van Straaten, G.); Stohr, A (Stoehr, A.); Link, S (Link, S.); Soubatch, S (Soubatch, S.); Jelinek, P (Jelinek, P.); Lee, TL (Lee, T-L); Starke, U (Starke, U.); Svec, M (Svec, M.); Bocquet, FC (Bocquet, F. C.); Tautz, FS (Tautz, F. S.)

Source: PHYSICAL REVIEW LETTERS **Volume:** 116 **Issue:** 12 **Article Number:** 126805 **DOI:** 10.1103/PhysRevLett.116.126805 **Published:** MAR 24 2016

Abstract: We investigate the structural and electronic properties of nitrogen-doped epitaxial monolayer graphene and quasifreestanding monolayer graphene on 6H-SiC(0001) by the normal incidence x-ray standing wave technique and by angle-resolved photoelectron spectroscopy supported by density functional theory simulations. With the location of various nitrogen species uniquely identified, we observe that for the same doping procedure, the graphene support, consisting of substrate and interface, strongly influences the structural as well as the electronic properties of the resulting doped graphene layer. Compared to epitaxial graphene, quasifreestanding graphene is found to contain fewer nitrogen dopants. However, this lack of dopants is compensated by the proximity of nitrogen atoms at the interface that yield a similar number of charge carriers in graphene.

Accession Number: WOS:000372729200014

PubMed ID: 27058093

Author Identifiers:

Author	ResearcherID Number	ORCID Number
van Straaten, Gerben	A-9680-2017	0000-0002-6004-5740
Bocquet, Francois	B-7845-2010	0000-0002-9471-4439
Jelinek, Pavel	G-1542-2010	0000-0002-5645-8542
Tautz, Frank Stefan	L-4500-2016	0000-0003-3583-2379
Svec, Martin	G-6645-2014	
Subach, Sergey		0000-0002-1455-0260
Franke, Markus		0000-0003-1168-5415

ISSN: 0031-9007

eISSN: 1079-7114

Record 303 of 491

Title: Thermodynamic Properties of Selected Homologous Series of Ionic Liquids Calculated Using Molecular Dynamics

Author(s): Cervinka, C (Cervinka, Ctirad); Padua, AAH (Padua, Agilio A. H.); Fulem, M (Fulem, Michal)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 120 **Issue:** 9 **Pages:** 2362-2371 **DOI:** 10.1021/acs.jpcb.5b11070 **Published:** MAR 10 2016

Abstract: This work presents a molecular dynamics simulation study concerning the thermodynamic data of ionic liquids (ILs) including phase change enthalpies, liquid phase densities, radial and spatial distribution functions, and diffusive properties. Three homologous series of ILs were selected for this study, namely, 1-alkyl-3-methylimidazolium tetrafluoroborates, hexafluorophosphates, and 1,1,2,2-tetrafluoroethanesulfonates, so that properties of 36 ILs are calculated in total. The trends of calculated properties are compared to available experimental data and thoroughly discussed in context of the homologous series. The calculated trends of the vaporization enthalpies within the series are supported by analyzing the structural properties of the ILs. An excellent agreement of calculated structural properties (liquid phase density) with the experimental counterparts is reached. The calculated enthalpic properties are overestimated considerably; thus, further development of the force fields for ILs is required.

Accession Number: WOS:000372042000032

PubMed ID: 26848831

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cervinka, Ctirad	L-8310-2017	0000-0003-1498-6715
Padua, Agilio	B-5126-2008	0000-0002-7641-6526
Fulem, Michal	B-7450-2008	0000-0002-5707-0670

ISSN: 1520-6106

Record 304 of 491

Title: Exact diagonalization study of the effects of Zn and Ni impurities on the pseudogap of underdoped cuprate high-T-c superconductors

Author(s): Vasatko, J (Vasatko, Jiri); Munzar, D (Munzar, Dominik)

Source: PHYSICAL REVIEW B **Volume:** 93 **Issue:** 9 **Article Number:** 094512 **DOI:** 10.1103/PhysRevB.93.094512 **Published:** MAR 9 2016

Abstract: The influence of Zn and Ni impurities on the normal-state pseudogap of underdoped high-T-c cuprate superconductors is studied using exact diagonalization of effective t-J-like Hamiltonians describing low energy electronic excitations of the CuO2 plane with some of the copper ions replaced with Zn/Ni. The Ni case Hamiltonian has been obtained by a sequence of approximations from a more complete model involving Cu 3d, Ni 3d, and O 2p orbitals. Our main findings are: (i) The width Omega(PG) of the pseudogap occurring in the many body density of states, and manifesting itself also in the c-axis infrared conductivity, decreases with increasing Zn concentration as a consequence of a suppression of short range spin correlations. (ii) In the case of one hole and one Ni impurity, the hole is-for realistic values of the model parameters-weakly bound to the Ni site. This causes a slight increase of Omega(PG) with respect to the pure case. (iii) Based on this result and further results for 1-2 holes and 1-2 Ni impurities, we suggest that in the real Ni substituted CuO2 plane Omega(PG) is larger than in the pure case due to the binding of the doped holes to the Ni sites and effective underdoping. Our findings clarify the trends observed in the c-axis infrared conductivity data of Zn and Ni substituted (Sm, Nd) Ba2Cu3O7-delta crystals.

Accession Number: WOS:000371729000007

ISSN: 2469-9950

eISSN: 2469-9969

Record 305 of 491

Title: Spectroscopic Characterization and Reactivity of Triplet and Quintet Iron(IV) Oxo Complexes in the Gas Phase

Author(s): Andris, E (Andris, Erik); Jasik, J (Jasik, Juraj); Gomez, L (Gomez, Laura); Costas, M (Costas, Miquel); Roithova, J (Roithova, Jana)

Source: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 55 **Issue:** 11 **Pages:** 3637-3641 **DOI:** 10.1002/anie.201511374 **Published:** MAR 7 2016

Abstract: Closely structurally related triplet and quintet iron(IV) oxo complexes with a tetradentate aminopyridine ligand were generated in the gas phase, spectroscopically characterized, and their reactivities in hydrogen-transfer and oxygen-transfer reactions were compared. The spin states were unambiguously assigned based on helium tagging infrared photodissociation (IRPD) spectra of the mass-selected iron complexes. It is shown that the stretching vibrations of the nitrate counterion can be used as a spectral marker of the central iron spin state.

Accession Number: WOS:000371521000015

PubMed ID: 26878833

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Laura, Gomez	F-7094-2016	0000-0003-3719-6855
Andris, Erik	O-2513-2017	0000-0002-9336-0157
Jasik, Juraj	O-1057-2017	0000-0002-1177-2837
costas, Miquel	H-6920-2012	0000-0001-6326-8299
Roithova, Jana		0000-0001-5144-0688

ISSN: 1433-7851

eISSN: 1521-3773

Record 306 of 491

Title: New results on reduced-round Tiny Encryption Algorithm using genetic programming

Author(s): Kubicek, K (Kubicek, Karel); Novotny, J (Novotny, Jiri); Svenda, P (Svenda, Petr); Ukrop, M (Ukrop, Martin)

Source: INFOCOMMUNICATIONS JOURNAL **Volume:** 8 **Issue:** 1 **Pages:** 2-9 **Published:** MAR 2016

Abstract: Analysis of cryptoprimitives usually requires extensive work of a skilled cryptanalyst. Some automation is possible, e.g. by using randomness testing batteries such as Statistical Test Suite from NIST (NIST STS) or Dieharder. Such batteries compare the statistical properties of the functions output stream to the theoretical values. A potential drawback is a limitation to predefined tested patterns. However, there is a new approach EACirc is a genetically inspired randomness testing framework based on finding a dynamically constructed test. This test works as a probabilistic distinguisher separating cipher outputs from truly random data.
In this work, we use EACirc to analyze the outputs of Tiny Encryption Algorithm (TEA). TEA was selected as a frequently used benchmark algorithm for cryptanalytic approaches based on genetic algorithms. In this paper, we provide results of EACirc applied to TEA ciphertext created from differently structured plaintext. We compare the methodology and results with previous approaches for limited-round TEA. A different construction of EACirc tests also allows us to determine which part of ciphers output is relevant to the decision of a well-performing randomness distinguisher.

Accession Number: WOS:000382864400002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Svenda, Petr	M-7619-2017	0000-0002-9784-7624
Ukrop, Martin		0000-0001-8110-8926

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Record 307 of 491

Title: DETECTION OF GRAPEVINE PINOT GRIS VIRUS IN CERTIFIED GRAPEVINE STOCKS IN MORAVIA, CZECH REPUBLIC

Author(s): Eichmeier, A (Eichmeier, A.); Penazova, E (Penazova, E.); Pavelkova, R (Pavelkova, R.); Mynarzova, Z (Mynarzova, Z.); Saldarelli, P (Saldarelli, P.)

Source: JOURNAL OF PLANT PATHOLOGY **Volume:** 98 **Issue:** 1 **Pages:** 155-157 **Published:** MAR 2016

Abstract: Twenty one grapevine mother plants used by nurseries for propagation in South Moravia, Czech Republic, were tested for the presence of Grapevine Pinot gris virus (GPGV) and other viruses by simplex and multiplex RTPCR. GPGV was found in all vines tested and Grapevine virus A, Grapevine fanleaf virus and Grapevine fleck virus were detected only in some of them. Part of the movement and coat protein coding regions of 21 GPGV isolates was sequenced. Phylogenetic analysis revealed that south Moravian GPGV isolates grouped with isolates from other regions and countries. This study provides the first comprehensive survey of the GPGV occurrence in South Moravia.

Accession Number: WOS:000375009900020

ISSN: 1125-4653

Record 308 of 491

Title: Discovery of Novel Haloalkane Dehalogenase Inhibitors

Author(s): Buryska, T (Buryska, Tomas); Daniel, L (Daniel, Lukas); Kunka, A (Kunka, Antonin); Brezovsky, J (Brezovsky, Jan); Damborsky, J (Damborsky, Jiri); Prokop, Z (Prokop, Zbynek)

Source: APPLIED AND ENVIRONMENTAL MICROBIOLOGY **Volume:** 82 **Issue:** 6 **Pages:** 1958-1965 **DOI:** 10.1128/AEM.03916-15 **Published:** MAR 2016

Abstract: Haloalkane dehalogenases (HLDs) have recently been discovered in a number of bacteria, including symbionts and pathogens of both plants and humans. However, the biological roles of HLDs in these organisms are unclear. The development of efficient HLD inhibitors serving as molecular probes to explore their function would represent an important step toward a better understanding of these interesting enzymes. Here we report the identification of inhibitors for this enzyme family using two different approaches. The first builds on the structures of the enzymes' known substrates and led to the discovery of less potent nonspecific HLD inhibitors. The second approach involved the virtual screening of 150,000 potential inhibitors against the crystal structure of an HLD from the human pathogen Mycobacterium tuberculosis H37Rv. The best inhibitor exhibited high specificity for the target structure, with an inhibition constant of 3 mu M and a molecular architecture that clearly differs from those of all known HLD substrates. The new inhibitors will be used to study the natural functions of HLDs in bacteria, to probe their mechanisms, and to achieve their stabilization.

Accession Number: WOS:000373339400032

PubMed ID: 26773086

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Prokop, Zbynek	H-5707-2012	
Damborsky, Jiri	H-3799-2012	0000-0002-7848-8216
Brezovsky, Jan	C-8290-2012	0000-0001-9677-5078
Daniel, Lukas		0000-0003-2502-9224
Prokop, Zbynek		0000-0001-9358-4081

ISSN: 0099-2240

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Record 309 of 491

Title: Engel-Vosko generalized gradient approximation within DFT investigations of optoelectronic and thermoelectric properties of copper thioantimonates(III) and thioarsenate(III) for solar-energy conversion

Author(s): Khan, W (Khan, Wilayat); Goumri-Said, S (Goumri-Said, Souraya)

Source: PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS **Volume:** 253 **Issue:** 3 **Pages:** 583-590 **DOI:** 10.1002/pssb.201552435 **Published:** MAR 2016

Abstract: The electronic structure and optical properties of Rb2Cu2Sb2S5, Cs2Cu2Sb2S5, and Rb8Cu6As8S19 were investigated from first principles based on Engel-Vosko generalized gradient approximation (EV-GGA). The calculated band structures and density of states confirm that these compounds have an indirect bandgap. The bands near the Fermi level were mainly contributed from Cu-3d states along with a small participation of S-3p states. The partial density of states shows that Cs and Rb elements are bonded ionically to sulfur, whereas Cu, Sb, As, and S element show covalent bonds with each other. From the electronic structure and using EV-GGA, the frequency-dependent optical parameters such as the real and imaginary parts of the dielectric functions, energy loss function, and reflectivity were calculated. These optical parameters prove that these compounds are potentially interesting for the field of optoelectronic and optical devices. The temperature-dependent thermoelectric properties such as the electrical conductivity, Seebeck coefficient, thermal conductivity, and power factor were calculated based on combination of DFT output and Boltzmann transport theory. (C) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

Accession Number: WOS:000371634800026
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862

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Record 310 of 491

Title: Distributed capillary adiabatic tissue homogeneity model in parametric multi-channel blind AIF estimation using DCE-MRI
Author(s): Kratochvila, J (Kratochvila, Jiri); Jirik, R (Jirik, Radovan); Bartos, M (Bartos, Michal); Standara, M (Standara, Michal); Starcuk, Z (Starcuk, Zenon, Jr.); Taxt, T (Taxt, Torfinn)
Source: MAGNETIC RESONANCE IN MEDICINE **Volume:** 75 **Issue:** 3 **Pages:** 1355-1365 **DOI:** 10.1002/mrm.25619 **Published:** MAR 2016
Abstract: PurposeOne of the main challenges in quantitative dynamic contrast-enhanced (DCE) MRI is estimation of the arterial input function (AIF). Usually, the signal from a single artery (ignoring contrast dispersion, partial volume effects and flow artifacts) or a population average of such signals (also ignoring variability between patients) is used. MethodsMulti-channel blind deconvolution is an alternative approach avoiding most of these problems. The AIF is estimated directly from the measured tracer concentration curves in several tissues. This contribution extends the published methods of multi-channel blind deconvolution by applying a more realistic model of the impulse residue function, the distributed capillary adiabatic tissue homogeneity model (DCATH). In addition, an alternative AIF model is used and several AIF-scaling methods are tested. ResultsThe proposed method is evaluated on synthetic data with respect to the number of tissue regions and to the signal-to-noise ratio. Evaluation on clinical data (renal cell carcinoma patients before and after the beginning of the treatment) gave consistent results. An initial evaluation on clinical data indicates more reliable and less noise sensitive perfusion parameter estimates. ConclusionBlind multi-channel deconvolution using the DCATH model might be a method of choice for AIF estimation in a clinical setup. Magn Reson Med 75:1355-1365, 2016. (c) 2015 Wiley Periodicals, Inc.
Accession Number: WOS:000370593700042
PubMed ID: 25865576
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Starcuk, Zenon	G-1233-2014	0000-0002-1218-0585
Jirik, Radovan	F-6226-2012	0000-0003-2555-9428
Bartos, Michal	H-8495-2014	0000-0003-4389-7703
Kratochvila, Jiri	D-8607-2015	

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Record 311 of 491

Title: Effect of TFE on the Helical Content of AK17 and HAL-1 Peptides: Theoretical Insights into the Mechanism of Helix Stabilization
Author(s): Vymetal, J (Vymetal, Jiri); Bednarova, L (Bednarova, Lucie); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 120 **Issue:** 6 **Pages:** 1048-1059 **DOI:** 10.1021/acs.jpcb.5b11228 **Published:** FEB 18 2016
Abstract: Fluorinated alcohols such as 2,2,2-trifluoroethanol (TFE) are among the most frequently used, cosolvents in experiment studies of peptides. They have significant effects on secondary structure and a particularly strong promotion of alpha-helix is induced by TFE. In this study we validated recently proposed force field parameters for TFE in molecular dynamics simulations with two model peptides-alanine-rich AK-17 and antimicrobial peptide halictine-1 (HAL-1). In the case of HAL-1, we characterized the effect of TFE on this peptide experimentally by ECD spectroscopy. Our TFE model in question reproduced the helix-promoting effect of TFE and provided insight into the mechanisms of TFE action on peptides. Our simulations confirmed the preferential interaction of TFE molecules with alpha-helices, although the TFE molecules accumulate in the vicinity of the peptides in various conformations. Moreover, we observed a significant effect of TFE on the thermodynamics of the helix-coil transition and a change in local conformational preferences in the unfolded (coil) state induced by TFE. In addition, our simulation-based analysis suggests that different mechanisms participate in helix stabilization in both model peptides in water and TFE solution. Our results thus support the picture of complex TFE action on peptides that is further diversified by the identity and intrinsic properties of the peptide.
Accession Number: WOS:000370678500002
PubMed ID: 26786280
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vondrasek, Jiri	A-4244-2008	
Vymetal, Jiri	R-1167-2017	0000-0002-0165-8707

ISSN: 1520-6106

Record 312 of 491

Title: Palladium clusters on graphene support: An ab initio study
Author(s): Rubes, M (Rubes, Miroslav); He, JJ (He, Junjie); Nachtigall, P (Nachtigall, Petr); Bludsky, O (Bludsky, Ota)
Source: CHEMICAL PHYSICS LETTERS **Volume:** 646 **Pages:** 56-63 **DOI:** 10.1016/j.cplett.2015.12.065 **Published:** FEB 16 2016
Abstract: CCSD(T) calculations with an energy-consistent scalar relativistic pseudopotential have been performed on a series of Pd-PAH complexes. The CCSD(T)//CBS interaction energies for Pd-ethylene and Pd-PAH (PAH = benzene, naphthalene, pyrene, coronene and ovalene) are -32.3, -25.3, -21.0, -22.5, -23.1 and -24.0 kcal mol(-1), respectively. A DFT/CC interaction model based on the Pd-PAH calculations has been proposed for a reliable and accurate description of Pd-cluster interaction with graphene support. PBE/CC and PBEh/CC calculations for Pd-n-PAH and Pd-n-graphene (n<4) are reported. The PBEh/CC value of -27.7 kcal mol(-1) is our best estimate of the Pd-graphene interaction energy. (C) 2016 Elsevier B.V. All rights reserved.
Accession Number: WOS:000369968900011
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bludsky, Ota	A-5659-2008	
Nachtigall, Petr	A-6220-2013	0000-0002-1628-7275
He, Junjie	O-6825-2017	0000-0001-6447-7893

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Record 313 of 491

Title: High-Frequency C-13 and Si-29 NMR Chemical Shifts in Diamagnetic Low-Valence Compounds of TII and Pb-II: Decisive Role of Relativistic Effects
Author(s): Vicha, J (Vicha, Jan); Marek, R (Marek, Radek); Straka, M (Straka, Michal)
Source: INORGANIC CHEMISTRY **Volume:** 55 **Issue:** 4 **Pages:** 1770-1781 **DOI:** 10.1021/acs.inorgchem.5b02689 **Published:** FEB 15 2016
Abstract: The C-13 and Si-29 NMR signals of ligand atoms directly bonded to TII or Pb-II heavy-element centers are predicted to resonate at very high frequencies, up to 400 ppm for C-13 and over 1000 ppm for Si-29, outside the typical experimental NMR chemical-shift ranges for a given type of nuclei. The large C-13 and Si-29 NMR chemical shifts are ascribed to sizable relativistic spin-orbit effects, which can amount to more than 200 ppm for C-13 and more than 1000 ppm for Si-29, values unexpected for diamagnetic compounds of the main group elements. The origin of the vast spin-orbit contributions to the C-13 and Si-29 NMR shifts is traced to the highly efficient 6p -> 6p* metal-based orbital magnetic couplings and related to the 6p orbital-based bonding together with the low-energy gaps between the occupied and virtual orbital subspaces in the subvalent TII and Pb-II compounds. New NMR spectral regions for these compounds are suggested based on the fully relativistic density functional theory calculations in the Dirac-Coulomb framework carefully calibrated on the experimentally known NMR data for TII and Pb-II complexes.
Accession Number: WOS:000370395000049

PubMed ID: 26820039
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Straka, Michal	E-5246-2011	0000-0002-7857-4990
Vicha, Jan	D-8417-2012	0000-0003-3698-8236
Marek, Radek	D-6929-2012	0000-0002-3668-3523

ISSN: 0020-1669
eISSN: 1520-510X

Record 314 of 491

Title: Synthesis, antimicrobial evaluation and molecular modeling of 5-hydroxyisoquinolinium salt series; the effect of the hydroxyl moiety
Author(s): Soukup, O (Soukup, Ondrej); Dolezal, R (Dolezal, Rafael); Malinak, D (Malinak, David); Marek, J (Marek, Jan); Salajkova, S (Salajkova, Sarka); Pasdiorova, M (Pasdiorova, Marketa); Honegr, J (Honegr, Jan); Korabecny, J (Korabecny, Jan); Nachtigal, P (Nachtigal, Petr); Nachon, F (Nachon, Florian); Jun, D (Jun, Daniel); Kuca, K (Kuca, Kamil)
Source: BIOORGANIC & MEDICINAL CHEMISTRY **Volume:** 24 **Issue:** 4 **Pages:** 841-848 **DOI:** 10.1016/j.bmc.2016.01.006 **Published:** FEB 15 2016
Abstract: In the present paper, we describe the synthesis of a new group of 5-hydroxyisoquinolinium salts with different lengths of alkyl side-chain (C-10-C-18), and their chromatographic analysis and biological assay for in vitro activity against bacterial and fungal strains. We compare the lipophilicity and efficacy of hydroxylated isoquinolinium salts with the previously published (non-hydroxylated) isoquinolinium salts from the point of view of antibacterial and antifungal versatility and cytotoxic safety. Compound 11 (C-18) had to be excluded from the testing due to its low solubility. Compounds 9 and 10 (C-14, C-16) showed only moderate efficacy against G+ bacteria, notably with excellent potency against Staphyloccocus aureus, but no effect against G- bacteria. In contrast, non-hydroxylated isoquinolinium salts showed excellent antimicrobial efficacy within the whole series, particularly 14 (C-14) against G+ strains and 15 (C-16) against fungi. The electronic properties and desolvation energies of 5-hydroxyisoquinolinium and isoquinolinium salts were studied by quantum-chemistry calculations employing B3LYP/6-311++G(d,p) method and an implicit water-solvent simulation model (SCRF). Despite the positive mesomeric effect of the hydroxyl moiety reducing the electron density of the quaternary nitrogen, it is probably the higher lipophilicity and lower desolvation energy of isoquinolinium salts, which is responsible for enhanced antimicrobial versatility and efficacy. (c) 2016 Elsevier Ltd. All rights reserved.
Accession Number: WOS:000368898500035
PubMed ID: 26774252
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dolezal, Rafael	B-3956-2017	
Honegr, Jan	B-4487-2010	0000-0002-9225-677X
Jun, Daniel	S-8647-2017	0000-0002-0882-6304
Nachtigal, Petr	S-8022-2017	0000-0001-9568-7295
Benkova, Marketa		0000-0002-9196-9073

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Record 315 of 491

Title: CCSD(T)/CBS fragment-based calculations of lattice energy of molecular crystals
Author(s): Cervinka, C (Cervinka, Ctirad); Fulem, M (Fulem, Michal); Ruzicka, K (Ruzicka, Kvetoslav)
Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 144 **Issue:** 6 **Article Number:** 064505 **DOI:** 10.1063/1.4941055 **Published:** FEB 14 2016
Abstract: A comparative study of the lattice energy calculations for a data set of 25 molecular crystals is performed using an additive scheme based on the individual energies of up to four-body interactions calculated using the coupled clusters with iterative treatment of single and double excitations and perturbative triples correction (CCSD(T)) with an estimated complete basis set (CBS) description. The CCSD(T)/CBS values on lattice energies are used to estimate sublimation enthalpies which are compared with critically assessed and thermodynamically consistent experimental values. The average absolute percentage deviation of calculated sublimation enthalpies from experimental values amounts to 13% (corresponding to 4.8 kJ mol(-1) on absolute scale) with unbiased distribution of positive to negative deviations. As pair interaction energies present a dominant contribution to the lattice energy and CCSD(T)/CBS calculations still remain computationally costly, benchmark calculations of pair interaction energies defined by crystal parameters involving 17 levels of theory, including recently developed methods with local and explicit treatment of electronic correlation, such as LCC and LCC-F12, are also presented. Locally and explicitly correlated methods are found to be computationally effective and reliable methods enabling the application of fragment-based methods for larger systems. (C) 2016 AIP Publishing LLC.
Accession Number: WOS:000371607800023
PubMed ID: 26874495
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ruzicka, Kvetoslav	B-1071-2008	0000-0001-9048-1036
Cervinka, Ctirad	L-8310-2017	0000-0003-1498-6715
Fulem, Michal	B-7450-2008	0000-0002-5707-0670

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Record 316 of 491

Title: Benchmark Theoretical and Experimental Study on N-15 NMR Shifts of Oxidatively Damaged Guanine
Author(s): Dracinsky, M (Dracinsky, Martin); Sala, M (Sala, Michal); Klepetarova, B (Klepetarova, Blanka); Sebera, J (Sebera, Jakub); Fukal, J (Fukal, Jiri); Holeckova, V (Holeckova, Veronika); Tanaka, Y (Tanaka, Yoshiyuki); Nencka, R (Nencka, Radim); Sychrovsky, V (Sychrovsky, Vladimir)
Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 120 **Issue:** 5 **Pages:** 915-925 **DOI:** 10.1021/acs.jpcb.5b11428 **Published:** FEB 11 2016
Abstract: The N-15 NMR shifts of 9-ethyl-8-oxoguanine (OG) were calculated and measured in liquid DMSO and in crystal. The OG molecule is a model for oxidatively damaged 2'-deoxyguanosine that occurs owing to oxidative stress in cell. The DNA lesion is repaired with human 8-oxoguanine glycosylase 1 (hOGG1) base-excision repair enzyme, however, the exact mechanism of excision of damaged nucleobase with hOGG1 is currently unknown. This benchmark study on N-15 NMR shifts of OG aims their accurate structural interpretation and calibration of the calculation protocol utilizable in future studies on mechanism of hOGG1 enzyme. The effects of NMR reference, DFT functional, basis set, solvent, structure, and dynamics on calculated N-15 NMR shifts were first evaluated for OG in crystal to calibrate the best performing calculation method. The effect of large-amplitude motions on N-15 NMR shifts of OG in liquid was calculated employing molecular dynamics. The B3LYP method with Iglo-III basis used for B3LYP optimized geometry with 6-311++G(d,p) basis and including effects of solvent and molecular dynamic was the calculation protocol used for calculation of N-15 NMR shifts of OG. The NMR shift of N9 nitrogen of OG was particularly studied because the atom is involved in an N-glycosidic bond that is cleaved with hOGG1. The change of N9 NMR shift owing to oxidation of 9-ethylguanine (G) measured in liquid was -27.1 ppm. The calculated N9 NMR shift of OG deviated from experiment in crystal and in liquid by 0.45 and 0.65 ppm, respectively. The calculated change of N9 NMR shift owing to notable N9-pyramidalization of OG in one previously found polymorph was 20.53 ppm. We therefore assume that the pyramidal geometry of N9 nitrogen that could occur for damaged DNA within hOGG1 catalytic site might be detectable with N-15 NMR spectroscopy. The calculation protocol can be used for accurate structural interpretation of N-15 NMR shifts of oxidatively damaged guanine DNA residue.
Accession Number: WOS:000370210600006
PubMed ID: 26727398
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sychrovsky, Vladimir	G-5558-2014	
Sebera, Jakub	B-6112-2013	0000-0001-5671-5206
Tanaka, Yoshiyuki	B-1730-2008	

Fukal, Jiri	S-7922-2017	0000-0002-0188-8828
Nencka, Radim	G-5296-2014	
Sala, Michal	H-2839-2014	

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Record 317 of 491

Title: Software Defined Monitoring of Application Protocols

Author(s): Kekely, L (Kekely, Lucas); Kucera, J (Kucera, Jan); Pus, V (Pus, Viktor); Korenek, J (Korenek, Jan); Vasilakos, AV (Vasilakos, Athanasios V.)

Source: IEEE TRANSACTIONS ON COMPUTERS **Volume:** 65 **Issue:** 2 **Pages:** 615-626 **DOI:** 10.1109/TC.2015.2423668 **Published:** FEB 2016

Abstract: With the ongoing shift of network services to the application layer also the monitoring systems focus more on the data from the application layer. The increasing speed of the network links, together with the increased complexity of application protocol processing, require a new way of hardware acceleration. We propose a new concept of hardware acceleration for flexible flow-based application level traffic monitoring which we call Software Defined Monitoring. Application layer processing is performed by monitoring tasks implemented in the software in conjunction with a configurable hardware accelerator. The accelerator is a high-speed application-specific processor tailored to stateful flow processing. The software monitoring tasks control the level of detail retained by the hardware for each flow in such a way that the usable information is always retained, while the remaining data is processed by simpler methods. Flexibility of the concept is provided by a plugin-based design of both hardware and software, which ensures adaptability in the evolving world of network monitoring. Our high-speed implementation using FPGA acceleration board in a commodity server is able to perform a 100 Gb/s flow traffic measurement augmented by a selected application-level protocol analysis.

Accession Number: WOS:000372753500021

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vasilakos, Athanasios	J-2824-2017	

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Record 318 of 491

Title: First principles studies on the impact of point defects on the phase stability of (AlxCr1-x)(2)O-3 solid solutions

Author(s): Koller, CM (Koller, C. M.); Koutna, N (Koutna, N.); Ramm, J (Ramm, J.); Kolozsvari, S (Kolozsvari, S.); Paulitsch, J (Paulitsch, J.); Holec, D (Holec, D.); Mayrhofer, PH (Mayrhofer, P. H.)

Source: AIP ADVANCES **Volume:** 6 **Issue:** 2 **Article Number:** 025002 **DOI:** 10.1063/1.4941573 **Published:** FEB 2016

Abstract: Density Functional Theory applying the generalised gradient approximation is used to study the phase stability of (AlxCr1-x)(2)O-3 solid solutions in the context of physical vapour deposition (PVD). Our results show that the energy of formation for the hexagonal a phase is lower than for the metastable cubic. and B1-like phases-independent of the Al content x. Even though this suggests higher stability of the a phase, its synthesis by physical vapour deposition is difficult for temperatures below 800 degrees C. Aluminium oxide and Al-rich oxides typically exhibit a multi-phased, cubic-dominated structure. Using a model system of (Al0.69Cr0.31)(2)O-3 which experimentally yields larger fractions of the desired hexagonal a phase, we show that point defects strongly influence the energetic relationships. Since defects and in particular point defects, are unavoidably present in PVD coatings, they are important factors and can strongly influence the stability regions. We explicitly show that defects with low formation energies (e.g. metal Frenkel pairs) are strongly preferred in the cubic phases, hence a reasonable factor contributing to the observed thermodynamically anomalous phase composition. (C) 2016 Author(s).

Accession Number: WOS:000371739000002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mayrhofer, Paul	A-9640-2011	0000-0001-7328-9333
Koller, Christian	H-3558-2017	0000-0003-0410-9364
Holec, David		0000-0002-3516-1061
Koutna, Nikola		0000-0001-7901-4736
Kolozsvari, Szilard		0000-0002-3397-7681

ISSN: 2158-3226

Record 319 of 491

Title: Set of rules for genomic signal downsampling

Author(s): Sedlar, K (Sedlar, Karel); Skutkova, H (Skutkova, Helena); Vitek, M (Vitek, Martin); Provaznik, I (Provaznik, Ivo)

Source: COMPUTERS IN BIOLOGY AND MEDICINE **Volume:** 69 **Pages:** 308-314 **DOI:** 10.1016/j.compbiomed.2015.05.022 **Published:** FEB 1 2016

Abstract: Comparison and classification of organisms based on molecular data is an important task of computational biology, since at least parts of DNA sequences for many organisms are available. Unfortunately, methods for comparison are computationally very demanding, suitable only for short sequences. In this paper, we focus on the redundancy of genetic information stored in DNA sequences. We proposed rules for downsampling of DNA signals of cumulated phase. According to the length of an original sequence, we are able to significantly reduce the amount of data with only slight loss of original information. Dyadic wavelet transform was chosen for fast downsampling with minimum influence on signal shape carrying the biological information. We proved the usability of such new short signals by measuring percentage deviation of pairs of original and downsampled signals while maintaining spectral power of signals. Minimal loss of biological information was proved by measuring the Robinson-Foulds distance between pairs of phylogenetic trees reconstructed from the original and downsampled signals. The preservation of inter-species and intra-species information makes these signals suitable for fast sequence identification as well as for more detailed phylogeny reconstruction. (C) 2015 The Authors. Published by Elsevier Ltd. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licensesiby-nc-nd/4.0/).

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PubMed ID: 26078051

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Skutkova, Helena	D-5194-2014	0000-0003-4562-2746
Provaznik, Ivo	F-4121-2012	0000-0002-3422-7938
Vitek, Martin	D-3351-2014	0000-0002-8059-1087
Sedlar, Karel	K-1120-2014	0000-0002-8269-4020

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Record 320 of 491

Title: STRUCTURAL CHANGES IN THE CZECH ECONOMY: A DSGE MODEL APPROACH

Author(s): Capek, J (Capek, Jan)

Source: PRAGUE ECONOMIC PAPERS **Volume:** 25 **Issue:** 1 **Pages:** 37-52 **Published:** FEB 2016

Abstract: This article identifies structural changes in the Czech economy in the period from 1996 to 2012 using a DSGE model estimated using Bayesian methods. A structural change is understood as a statistically significant change in model parameter(s).
Prior to the first quarter of 1999, there was a structural change that can be primarily attributed to shocks impacting only the domestic economy, and to the domestic monetary authority's increased preferences towards inflation and exchange rate growth. The elasticity of substitution between domestic and imported consumption goods also increased sharply in this period. As far as the recent economic recession is concerned, it was caused by a much more persistent worldwide technology shock. Habit formation dropped abruptly during the crisis as households tended not to smooth their consumption much anymore.
Recursive impulse response analysis carried out on the model suggests that the propagation mechanisms in the model economy changed, implying that the identified structural changes were accompanied by a change in behaviour of the model economy.

Accession Number: WOS:000371374000003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Capek, Jan	H-3581-2013	0000-0001-7640-5272

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Record 321 of 491
Title: Conformational Interconversions of Amino Acid Derivatives
Author(s): Kaminsky, J (Kaminsky, Jakub); Jensen, F (Jensen, Frank)
Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 12 **Issue:** 2 **Pages:** 694-705 **DOI:** 10.1021/acs.jctc.5b00911 **Published:** FEB 2016
Abstract: Exhaustive conformational interconversions including transition structure analyses of N-acetyl-L-glycine-N-methylamide as well as its alanine, serine, and cysteine analogues have been investigated at the MP2/6-31G** level, yielding a total of 142 transition states. Improved estimates of relative energies were obtained by separately extrapolating the Hartree-Fock and MP2 energies to the basis set limit and adding the difference between CCSD(T) and MP2 results with the cc-pVDZ basis set to the extrapolated MP2 results. The performance of eight empirical force fields (AMBER94, AMBER14SB, MM2, MM3, MMFFs, CHARMM22_CMAP, OPLS_2005, and AMOEBAPRO13) in reproducing ab initio energies of transition states was tested. Our results indicate that commonly used class I force fields employing a fixed partial charge model for the electrostatic interaction provide mean errors in the similar to 10 kJ/mol range for energies of conformational transition states for amino acid conformers. Modern reparametrized versions, such as CHARMM22_CMAP, and polarizable force fields, such as AMOEBAPRO13, have slightly lower mean errors, but maximal errors are still in the 35 kJ/mol range. There are differences between the force fields in their ability for reproducing conformational transitions classified according to backbone/side-chain or regions in the Ramachandran angles, but the data set is likely too small to draw any general conclusions. Errors in conformational interconversion barriers by similar to 10 kJ/mol suggest that the commonly used force field may bias certain types of transitions by several orders of magnitude in rate and thus lead to incorrect dynamics in simulations. It is therefore suggested that information for conformational transition states should be included in parametrization of new force fields.
Accession Number: WOS:000370112900022
PubMed ID: 26691979
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022
Jensen, Frank	A-2809-2017	0000-0002-4576-5838

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Record 322 of 491
Title: Allium telomeres unmasked: the unusual telomeric sequence (CTCGGTTATGGG)(n) is synthesized by telomerase
Author(s): Fajkus, P (Fajkus, Petr); Peska, V (Peska, Vratislav); Sitova, Z (Sitova, Zdenka); Fulneckova, J (Fulneckova, Jana); Dvorackova, M (Dvorackova, Martina); Gogela, R (Gogela, Roman); Sykorova, E (Sykorova, Eva); Hapala, J (Hapala, Jan); Fajkus, J (Fajkus, Jiri)
Source: PLANT JOURNAL **Volume:** 85 **Issue:** 3 **Pages:** 337-347 **DOI:** 10.1111/tpj.13115 **Published:** FEB 2016
Abstract: Phylogenetic divergence in Asparagales plants is associated with switches in telomere sequences. The last switch occurred with divergence of the genus Allium (Amaryllidaceae) from the other Allioideae (formerly Alliaceae) genera, resulting in uncharacterized telomeres maintained by an unknown mechanism. To characterize the unknown Allium telomeres, we applied a combination of bioinformatic processing of transcriptomic and genomic data with standard approaches in telomere biology such as BAL31 sensitivity tests, terminal restriction fragment analysis, the telomere repeat amplification protocol (TRAP), and fluorescence insitu hybridization (FISH). Using these methods, we characterize the unusual telomeric sequence (CTCGGTTATGGG)(n) present in Allium species, demonstrate its synthesis by telomerase, and characterize the telomerase reverse transcriptase (TERT) subunit of Allium cepa. Our findings open up the possibility of studying the molecular details of the evolutionary genetic change in Allium telomeres and its possible role in speciation. Experimental studies addressing the implications of this change in terms of the interplay of telomere components may now be designed to shed more light on telomere functions and evolution in general.
Accession Number: WOS:000369857400001
PubMed ID: 26716914
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fajkus, Jiri	D-2499-2012	0000-0002-3112-1716
Sykorova, Eva	D-9118-2012	0000-0002-4048-034X
Peska, Vratislav		0000-0002-0526-2988
Hapala, Jan		0000-0003-0568-5806

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Record 323 of 491
Title: A role for palindromic structures in the cis-region of maize Sirevirus LTRs in transposable element evolution and host epigenetic response
Author(s): Bousios, A (Bousios, Alexandros); Diez, CM (Diez, Concepcion M.); Takuno, S (Takuno, Shohei); Bystry, V (Bystry, Vojtech); Darzentas, N (Darzentas, Nikos); Gaut, BS (Gaut, Brandon S.)
Source: GENOME RESEARCH **Volume:** 26 **Issue:** 2 **Pages:** 226-237 **DOI:** 10.1101/gr.193763.115 **Published:** FEB 2016
Abstract: Transposable elements (TEs) proliferate within the genome of their host, which responds by silencing them epigenetically. Much is known about the mechanisms of silencing in plants, particularly the role of siRNAs in guiding DNA methylation. In contrast, little is known about siRNA targeting patterns along the length of TEs, yet this information may provide crucial insights into the dynamics between hosts and TEs. By focusing on 6456 carefully annotated, full-length Sirevirus LTR retro-transposons in maize, we show that their silencing associates with underlying characteristics of the TE sequence and also uncover three features of the host-TE interaction. First, siRNA mapping varies among families and among elements, but particularly along the length of elements. Within the cis-regulatory portion of the LTRs, a complex palindrome-rich region acts as a hotspot of both siRNA matching and sequence evolution. These patterns are consistent across leaf, tassel, and immature ear libraries, but particularly emphasized for floral tissues and 21-to 22-nt siRNAs. Second, this region has the ability to form hairpins, making it a potential template for the production of miRNA-like, hairpin-derived small RNAs. Third, Sireviruses are targeted by siRNAs as a decreasing function of their age, but the oldest elements remain highly targeted, partially by siRNAs that cross-map to the youngest elements. We show that the targeting of older Sireviruses reflects their conserved palindromes. Altogether, we hypothesize that the palindromes aid the silencing of active elements and influence transposition potential, siRNA targeting levels, and ultimately the fate of an element within the genome.
Accession Number: WOS:000369341900008
PubMed ID: 26631490
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bousios, Alexandros		0000-0002-8005-6949

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Record 324 of 491
Title: Ab initio study of energetics and magnetism of sigma phase in Co-Mo and Fe-Mo systems
Author(s): Pavlu, J (Pavlu, J.); Vrest'al, J (Vrest'al, J.); Sob, M (Sob, M.)
Source: MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING **Volume:** 24 **Issue:** 2 **Article Number:** 025009 **DOI:** 10.1088/0965-0393/24/2/025009 **Published:** FEB 2016

Abstract: We analyse, from first-principles, the energetics and magnetic ordering of sigma phases in Co-Mo and Fe-Mo systems. Total energy differences between the sigma phase and Standard Element Reference (SER) structures are calculated in the whole concentration range at equilibrium volumes by means of the linear muffin-tin orbitals method in the atomic-sphere approximation (LMTO-ASA), the full-potential linearised augmented-plane waves (FLAPW) method and the pseudopotential approach. They are compared with the enthalpy of formation of sigma phase obtained from the phase equilibria calculations at higher temperature based on the semiempirical CALPHAD (CALculation of PHAse Diagram) method. It turns out that the binary sigma phases are more stable than the weighted average of the sigma phase of elemental constituents and that this stability for Fe-Mo is higher than for Co-Mo. On the other hand it was found that the binary sigma phases do not exhibit any stability with respect to the weighted average of the SER structures. The magnetic configurations in all systems are investigated and the stabilizing effect of magnetic order in sigma phase at 0 K is presented. It turns out that the atomic magnetic moment strongly depends on the type of occupied sublattice and total composition of the alloy.

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Record 325 of 491

Title: Perturbation theory for an Anderson quantum dot asymmetrically attached to two superconducting leads

Author(s): Zonda, M (Zonda, M.); Pokorny, V (Pokorny, V.); Janis, V (Janis, V.); Novotny, T (Novotny, T.)

Source: PHYSICAL REVIEW B **Volume:** 93 **Issue:** 2 **Article Number:** 024523 **DOI:** 10.1103/PhysRevB.93.024523 **Published:** JAN 29 2016

Abstract: Self-consistent perturbation expansion up to the second order in the interaction strength is used to study a single-level quantum dot with local Coulomb repulsion attached asymmetrically to two generally different superconducting leads. At zero temperature and a wide range of other parameters, the spin-symmetric version of the expansion yields excellent results for the position of the 0-pi impurity quantum phase transition boundary and Josephson current together with the energy of Andreev bound states in the 0 phase as confirmed by numerical calculations using the numerical renormalization group method. We analytically prove that the method is charge conserving as well as thermodynamically consistent. Explicit formulas for the position of the 0-pi phase boundary are presented for the Hartree-Fock approximation as well as for its variant called generalized atomic limit. It is shown that the generalized atomic limit can be used as a quick estimate for the position of the phase boundary at half-filling in a broad range of parameters. We apply our second-order perturbation method to the interpretation of the existing experimental data on the phase boundary with very satisfactory outcome, suggesting that the so-far employed heavy numerical tools such as numerical renormalization group and/or quantum Monte Carlo are not necessary in a class of generic situations and can be safely replaced by a perturbative approach.

Accession Number: WOS:000369219600003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zonda, Martin	M-9520-2015	0000-0002-8513-3392
Pokorny, Vladislav	G-5750-2014	0000-0002-8944-6417
Novotny, Tomas	C-7392-2009	0000-0001-7014-4155
Janis, Vaclav	A-8379-2011	0000-0001-5959-6935

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Record 326 of 491

Title: E. coli metabolic protein aldehyde-alcohol dehydrogenase-E binds to the ribosome: a unique moonlighting action revealed

Author(s): Shasmal, M (Shasmal, Manidip); Dey, S (Dey, Sandip); Shaikh, TR (Shaikh, Tanvir R.); Bhakta, S (Bhakta, Sayan); Sengupta, J (Sengupta, Jayati)

Source: SCIENTIFIC REPORTS **Volume:** 6 **Article Number:** 19936 **DOI:** 10.1038/srep19936 **Published:** JAN 29 2016

Abstract: It is becoming increasingly evident that a high degree of regulation is involved in the protein synthesis machinery entailing more interacting regulatory factors. A multitude of proteins have been identified recently which show regulatory function upon binding to the ribosome. Here, we identify tight association of a metabolic protein aldehyde-alcohol dehydrogenase E (AdhE) with the E. coli 70S ribosome isolated from cell extract under low salt wash conditions. Cryo-EM reconstruction of the ribosome sample allows us to localize its position on the head of the small subunit, near the mRNA entrance. Our study demonstrates substantial RNA unwinding activity of AdhE which can account for the ability of ribosome to translate through downstream of at least certain mRNA helices. Thus far, in E. coli, no ribosome-associated factor has been identified that shows downstream mRNA helicase activity. Additionally, the cryo-EM map reveals interaction of another extracellular protein, outer membrane protein C (OmpC), with the ribosome at the peripheral solvent side of the 50S subunit. Our result also provides important insight into plausible functional role of OmpC upon ribosome binding. Visualization of the ribosome purified directly from the cell lysate unveils for the first time interactions of additional regulatory proteins with the ribosome.

Accession Number: WOS:000369055500001

PubMed ID: 26822933

ISSN: 2045-2322

Record 327 of 491

Title: Simulation of Raman optical activity of multi-component monosaccharide samples

Author(s): Melcrova, A (Melcrova, Adela); Kessler, J (Kessler, Jiri); Bour, P (Bour, Petr); Kaminsky, J (Kaminsky, Jakub)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 3 **Pages:** 2130-2142 **DOI:** 10.1039/c5cp04111b **Published:** JAN 21 2016

Abstract: Determination of the saccharide structure in solution is a laborious process that can be significantly enhanced by optical spectroscopies. Raman optical activity (ROA) spectra are particularly sensitive to the chirality and conformation. However, the interpretation of them is largely dependent on computational tools providing a limited precision only. To understand the limitations and the link between spectral shapes and the structure, in the present study we measured and interpreted using a combination of molecular dynamics (MD) and density functional theory (DFT) Raman and ROA spectra of glucose and mannose solutions. Factors important for analyses of mixtures of conformers, anomers, and different monosaccharides are discussed as well. The accuracy of the simulations was found to be strongly dependent on the quality of the hydration model; the dielectric continuum solvent model provided lower accuracy than averaging of many solvent-solute clusters. This was due to different conformer weighting rather than direct involvement of water molecules in scattering recorded as ROA. However, the cluster-based simulations also failed to correctly reproduce the ratios of principal monosaccharide forms. The best results were obtained by a combined MD/DFT simulation, with the ratio of a-and beta-anomers and the -CH2OH group rotamers determined experimentally by NMR. Then a decomposition of experimental spectra into calculated subspectra provided realistic results even for the glucose and mannose mixtures. Raman spectra decomposition provided a better overall accuracy (similar to 5%) than ROA (similar to 10%). The combination of vibrational spectroscopy with theoretical simulations represents a powerful tool for analysing the saccharide structure. Conversely, the ROA and Raman data can be used to verify the quality of MD force fields and other parameters of computational modeling.

Accession Number: WOS:000369482100086

PubMed ID: 26689801

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022
Bour, Petr	G-5561-2014	
Melcrova, Adela	D-4036-2016	0000-0001-6390-0522
Kessler, Jiri	G-2880-2012	0000-0001-6307-4339

ISSN: 1463-9076

eISSN: 1463-9084

Record 328 of 491

Title: On the possibility of excitonic magnetism in Ir double perovskites

Author(s): Pajskr, K (Pajskr, K.); Novak, P (Novak, P.); Pokorny, V (Pokorny, V.); Kolorenc, J (Kolorenc, J.); Arita, R (Arita, R.); Kunes, J (Kunes, J.)

Source: PHYSICAL REVIEW B **Volume:** 93 **Issue:** 3 **Article Number:** 035129 **DOI:** 10.1103/PhysRevB.93.035129 **Published:** JAN 21 2016

Abstract: We combine several numerical and semianalytical methods to study the 5d double perovskites Sr2YIrO6 and Ba2YIrO6, which were recently proposed to exhibit excitonic magnetism. Starting from the density-functional theory and the constrained random-phase approximation, we construct effective multiband Hubbard models. These are analyzed by means of static and dynamical mean-field theories and strong-coupling expansion. We find both materials to be insulators, but, contrary to the experimental claims, with a large spin gap of several hundreds of meV preventing the formation of an ordered state at low temperature.

Accession Number: WOS:000368485700007

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kunes, Jan	B-4484-2008	0000-0001-9682-7640
Arita, Ryotaro	D-5965-2012	0000-0001-5725-072X
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302
Pokorny, Vladislav	G-5750-2014	0000-0002-8944-6417

ISSN: 2469-9950

eISSN: 2469-9969

Record 329 of 491

Title: The variation of PbTiO3 bandgap at ferroelectric phase transition

Author(s): Zelezny, V (Zelezny, V.); Chvostova, D (Chvostova, D.); Simek, D (Simek, D.); Maca, F (Maca, F.); Masek, J (Masek, J.); Setter, N (Setter, N.); Huang, YH (Huang, Yu Hong)

Source: JOURNAL OF PHYSICS-CONDENSED MATTER **Volume:** 28 **Issue:** 2 **Article Number:** 025501 **DOI:** 10.1088/0953-8984/28/2/025501 **Published:** JAN 20 2016

Abstract: Optical properties of the PbTiO3 thin films fabricated by chemical solution deposition have been measured with variable angle spectroscopic ellipsometry in the spectral range of 1-6 eV and in the temperature interval from room temperature to 950 K. The optical response functions and band gap energy were determined in the whole temperature range. The direct band gap varies from the value 3.88 eV at room temperature to the value 3.67 eV just above the phase transition. The temperature dependence of the film lattice parameters was also measured by x-ray and it shows a strong correlation with the band gap. The comparison of experimental data with ab initio electronic structure calculations simulating the temperature development of dielectric function and band gap is also presented.

Accession Number: WOS:000368724600009

PubMed ID: 26678862

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Maca, Frantisek	G-4467-2014	

ISSN: 0953-8984

eISSN: 1361-648X

Record 330 of 491

Title: Transformation of metallic boron into substitutional dopants in graphene on 6H-SiC(0001)

Author(s): Sforzini, J (Sforzini, J.); Telychko, M (Telychko, M.); Krejci, O (Krejci, O.); Vondracek, M (Vondracek, M.); Svec, M (Svec, M.); Bocquet, FC (Bocquet, F. C.); Tautz, FS (Tautz, F. S.)

Source: PHYSICAL REVIEW B **Volume:** 93 **Issue:** 4 **Article Number:** 041302 **DOI:** 10.1103/PhysRevB.93.041302 **Published:** JAN 19 2016

Abstract: We investigate the development of the local bonding and chemical state of boron atoms during the growth of B-doped graphene on 6H-SiC(0001). Photoemission experiments reveal the presence of two chemical states, namely, boron in the uppermost SiC bilayers and boron substituted in both the graphene and buffer layer lattices. We demonstrate the participation of the dopant in the pi electron system of graphene by the presence of the pi* resonance in the near edge x-ray adsorption fine structure (NEXAFS) recorded at the BK-edge. The experimental findings are supported by NEXAFS simulations.

Accession Number: WOS:000368486600002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Svec, Martin	G-6645-2014	
Tautz, Frank Stefan	L-4500-2016	0000-0003-3583-2379
Krejci, Ondrej	G-5918-2014	0000-0002-4948-4312
Bocquet, Francois	B-7845-2010	0000-0002-9471-4439

ISSN: 1098-0121

eISSN: 1550-235X

Record 331 of 491

Title: Reduction Process of Tetraplatin in the Presence of Deoxyguanosine Monophosphate (dGMP): A Computational DFT Study

Author(s): Sebesta, F (Sebesta, Filip); Burda, JV (Burda, Jaroslav V.)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 22 **Issue:** 3 **Pages:** 1037-1047 **DOI:** 10.1002/chem.201503555 **Published:** JAN 18 2016

Abstract: The reduction mechanism of [Pt-IV(dach)Cl-4] (dach=diaminocyclohexyl) in the presence of dGMP was studied. The first step is substitution of a chloro ligand by dGMP, followed by nucleophilic attack of a phosphate or sugar oxygen atom to the C8-position of guanine. Subsequent reduction forms the [Pt-II(dach)Cl-2] complex. The whole process is completed by a hydrolysis. Two different pathways for the substitution reaction were examined: a direct associative and a Basolo-Pearson autocatalytic mechanism. All the explored structures were optimized at the B3LYP-D3/6-31G(d) level and by using the COSMO solvation model with Klamt's radii. Single-point energetics was determined at the B3LYP-GD3BJ/6-311+ +G(2df,2pd)/PCM/scaled-UAKS level. Activation barriers were used for an estimation of the rate constants and these were compared with experimental values. It was found that the rate-determining step is the nucleophilic attack with a slightly faster performance in the 3'-dGMP branch than in the case of 5'-dGMP with activation barriers of 21.1 and 20.4 kcal mol(-1) (experimental: 23.8 and 23.2 kcal mol(-1)). The reduction reaction is connected with an electron flow from guanine. The product of the reduction reaction is a chelate structure, which dissociates within the last reaction step, that is, a hydrolysis reaction. The whole redox process (substitution, reduction, and hydrolysis) is exergonic by 34 and 28 kcal mol(-1) for 5'-dGMP and 3'-dGMP, respectively.

Accession Number: WOS:000368906200026

PubMed ID: 26663432

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Burda, Jaroslav	C-9199-2009	0000-0001-9909-8797

ISSN: 0947-6539

eISSN: 1521-3765

Record 332 of 491

Title: Osmotic pressure of aqueous electrolyte solutions via molecular simulations of chemical potentials: Application to NaCl

Author(s): Smith, WR (Smith, William R.); Moucka, F (Moucka, Filip); Nezbeda, I (Nezbeda, Ivo)

Source: FLUID PHASE EQUILIBRIA **Volume:** 407 **Special Issue:** SI **Pages:** 76-83 **DOI:** 10.1016/j.fluid.2015.05.012 **Published:** JAN 15 2016

Abstract: The osmotic pressure, Pi, is an important thermodynamic property of aqueous electrolyte solutions, which is intimately related to the activity of the water solvent, and is sensitive to the details of the force field used in molecular simulations of such systems. Its calculation in the most important case of discrete water models has received scant attention in the literature; the only existing method involves a special-purpose molecular dynamics approach implementing virtual semi-permeable membranes separating solution and solvent phases. Here, we develop and demonstrate a new thermodynamically based approach utilizing simulation results for the salt chemical potential, mu(s), and for the solution specific volume, v(m). The methodology may also be used in principle to calculate the activity of water and of the electrolyte from simulation data for Pi and v(m). We demonstrate our approach in the case of aqueous NaCl solutions at ambient conditions by calculating new results for both Pi and the related osmotic coefficient property, phi, from simulation data for a mu(NaCl). We compare with experimental data the predictions of two polarizable force fields (AH/BK3 and AH/SWM4-DP) and of a typical non-polarizable force field (JC). We find that AH/BK3 produces results in good agreement with experiment for both Pi and phi over the entire experimentally accessible concentration range, and that the AH/SWM4-DP results are generally poor. The JC results are very good at concentrations below about 3 molal, but deteriorate rapidly at higher concentrations. (C) 2015 Elsevier B.V. All rights reserved.

Accession Number: WOS:000364894600007

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Moucka, Filip	M-4013-2013	0000-0002-1400-7890

ISSN: 0378-3812
eISSN: 1879-0224

Record 333 of 491
Title: Voting Detector: A Combination of Anomaly Detectors to Reveal Annotation Errors in TTS Corpora
Author(s): Matousek, J (Matousek, Jindrich); Tihelka, D (Tihelka, Daniel)
Book Group Author(s): Int Speech Commun Assoc
Source: 17TH ANNUAL CONFERENCE OF THE INTERNATIONAL SPEECH COMMUNICATION ASSOCIATION (INTERSPEECH 2016), VOLS 1-5: UNDERSTANDING SPEECH PROCESSING IN HUMANS AND MACHINES **Book Series:** Interspeech **Pages:** 1560-1564 **DOI:** 10.21437/Interspeech.2016-442 **Published:** 2016
Abstract: Anomaly detection techniques were shown to help in detecting word-level annotation errors in read-speech corpora for text to -speech synthesis. In this framework, correctly annotated words are considered as normal examples on which the detection methods are trained. Misannotated words are then taken as anomalous examples which do not conform to normal patterns of the trained detection models. In this paper we propose a concept of a voting detector a combination of anomaly detectors in which each "single" detector "votes" on whether a testing word is annotated correctly or not. The final decision is then made by aggregating the votes. Our experiments show that voting detector has a potential to overcome each of the single anomaly detectors.
Accession Number: WOS:000409394401007
Conference Title: 17th Annual Conference of the International-Speech-Communication-Association (INTERSPEECH 2016)
Conference Date: SEP 08-12, 2016
Conference Location: San Francisco, CA
Conference Sponsors: apple, amazon alexa, Google, Microsoft, ebay, facebook, YAHOO JAPAN, Baidu Res, IBM Res, CIRRUS LOGIC, DATATANG, NUANCE, Speechocean Ltd, Yandex, Raytheon Technol
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Matousek, Jindrich	C-2146-2011	0000-0002-7408-7730

ISSN: 2308-457X
ISBN: 978-1-5108-3313-5

Record 334 of 491
Title: Metal-Oxygen Hybridization and Core-Level Spectra in Actinide and Rare-Earth Oxides
Author(s): Kolorenc, J (Kolorenc, Jindrich)
Source: MRS ADVANCES **Volume:** 1 **Issue:** 44 **Pages:** 3007-3012 **DOI:** 10.1557/adv.2016.403 **Published:** 2016
Abstract: We employ a combination of the density-functional theory and the dynamical mean-field theory to study the electronic structure of selected rare-earth sesquioxides and dioxides. We concentrate on the core-level photoemission spectra, in particular, we illustrate how these spectra reflect the integer or fractional filling of the 4f orbitals. We compare the results to our earlier calculations of actinide dioxides and analyze why the core-level spectra of actinide compounds display a substantially reduced sensitivity to the filling of the 5f orbitals.
Accession Number: WOS:000412658300006
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302

ISSN: 2059-8521

Record 335 of 491
Title: COMPARISON OF AXIAL FAN ROTOR EXPERIMENTAL DATA WITH CFD SIMULATION
Author(s): Prachar, A (Prachar, Ales)
Source: ACTA POLYTECHNICA **Volume:** 56 **Issue:** 1 **Pages:** 62-66 **DOI:** 10.14311/APP.2016.56.0062 **Published:** 2016
Abstract: Data obtained from an experimental simulation on a new test rig for axial fans are compared to a CFD simulation. The Edge solver is used and the development needed for the simulation (boundary conditions, free stream consistency) is described. Adequate agreement between the measured and calculated data is observed.
Accession Number: WOS:000411572200009
ISSN: 1210-2709

Record 336 of 491
Title: Fisher Vectors in PLDA Speaker Verification System
Author(s): Zajic, Z (Zajic, Zbynek); Hruz, M (Hruz, Marek)
Edited by: Baozong Y; Qiuqi R; Yao Z; Gaoyun AN
Source: PROCEEDINGS OF 2016 IEEE 13TH INTERNATIONAL CONFERENCE ON SIGNAL PROCESSING (ICSP 2016) **Book Series:** International Conference on Signal Processing **Pages:** 1339-1342 **Published:** 2016
Abstract: The goal of this paper is to examine the Fisher Vector and incorporate this vector in the PLDA based speaker verification system. The PLDA based system utilizes the Supervector of Statistics extracted from a Gaussian Mixture Model (adopted from the speaker adaptation task) to collect the information about a speaker from a dataset. We compare the efficiency of the PLDA based speaker verification system using Supervector of Statistics and the same system with Fisher vector. The experimental results of these two approaches to the verification task and the fusion of these two systems indicate that the Fisher Vector brings almost the same information to the PLDA verification process as the Supervector of Statistics when sufficient data are available.
Accession Number: WOS:000406056300260
Conference Title: 13th IEEE International Conference on Signal Processing (ICSP)
Conference Date: NOV 06-10, 2016
Conference Location: Chengdu, PEOPLES R CHINA
Conference Sponsors: IEEE, Inst Engn & Technol, Union Radio Sci Int, Chinese Inst Elect, Beijing Jiaotong Univ, Int Conf Signal Proc, IEEE Beijing Sect, IET Beijing Local Network, Natl Nat Sci Fdn China, CIE Signal Proc Soc, IEEE Signal Proc Soc Beijing Chapter, IEEE Comp Soc Beijing Chapter, Japan China Sci & Technol Exchange Assoc, Shenzhen Univ, Intelligent Informat Inst, CIC Commun & Signal Proc Soc, Univ Minist Educ China, Program Innovat Res Team
ISSN: 2164-5221
ISBN: 978-1-5090-1345-6

Record 337 of 491
Title: NEMEA: A Framework for Network Traffic Analysis
Author(s): Cejka, T (Cejka, Tomas); Bartos, V (Bartos, Vaclav); Svepes, M (Svepes, Marek); Rosa, Z (Rosa, Zdenek); Kubatova, H (Kubatova, Hana)
Edited by: Limam N; Cheriet M; Zhani MF; Festor O; KeithMarsoun S; DosSantos CRP
Source: 2016 12TH INTERNATIONAL CONFERENCE ON NETWORK AND SERVICE MANAGEMENT AND WORKSHOPS(CNSM 2016) **Book Series:** International Conference on Network and Service Management **Pages:** 195-201 **Published:** 2016
Abstract: Since network attacks become more sophisticated, it is difficult to discover them using traditional analysis tools. For some kinds of attacks, it is necessary to analyze Application Layer (L7) information in order to detect them. However, there is a lack of existing tools capable of L7 processing and manipulation. Therefore, we propose a Clow-based modular Network Measurements Analysis (NEMEA) system to overcome the situation. NEMEA is designed with respect to a stream-wise concept, i.e. data are analyzed continuously in memory with minimal data storage. NEMEA is developed as an open-source project and is publicly available for world-wide community. It is designed for both experimental and operational use. It is able to process offline traffic traces as well as live network flows. The system is very flexible and can be easily extended by new modules. The modules are developed within a NEMEA framework that is a key component of the project. NEMEA thus represents a unified platform for research and development of new traffic

analysis methods. It covers several important topics not limited to analysis and detection. Originally, NEMEA has been developed for the purposes of Czech National Research and Education Network operator. Therefore, it is focused on handling high speed network traffic with links working at 100 Gbps.

Accession Number: WOS:000403950600024

Conference Title: 12th IEEE/IFIP/ACM International Conference on Network and Service Management (CNSM)

Conference Date: OCT 31-NOV 04, 2016

Conference Location: Ecole Technologie Superiere, Montreal, CANADA

Conference Sponsors: ACM, ACM SIGCOMM, IEEE, IFIP, IEEE Commun Soc, Distributed Management Task Force Inc, IBM, IEEE Software Defined Networks, IEEE Green ICT, IEEE Big Data

Conference Host: Ecole Technologie Superiere

ISSN: 2165-9605

ISBN: 978-3-901882-85-2

Record 338 of 491

Title: Building a Feedback Loop to Capture Evidence of Network Incidents

Author(s): Rosa, Z (Rosa, Zdenek); Cejka, T (Cejka, Tomas); Zadnik, M (Zadnik, Martin); Pus, V (Pus, Viktor)

Edited by: Limam N; Cheriet M; Zhani MF; Festor O; KeithMarsoun S; DosSantos CRP

Source: 2016 12TH INTERNATIONAL CONFERENCE ON NETWORK AND SERVICE MANAGEMENT AND WORKSHOPS(CNSM 2016) **Book Series:** International Conference on Network and Service Management **Pages:** 292-296 **Published:** 2016

Abstract: Flow measurement is extremely useful in network management, however, in some cases it is vital to observe the packets in full detail. To this end, we propose combining flow measurement, packet capture and network behavioral analysis. The evaluation of the proposed system shows its feasibility even in high-speed network environment.

Accession Number: WOS:000403950600042

Conference Title: 12th IEEE/IFIP/ACM International Conference on Network and Service Management (CNSM)

Conference Date: OCT 31-NOV 04, 2016

Conference Location: Ecole Technologie Superiere, Montreal, CANADA

Conference Sponsors: ACM, ACM SIGCOMM, IEEE, IFIP, IEEE Commun Soc, Distributed Management Task Force Inc, IBM, IEEE Software Defined Networks, IEEE Green ICT, IEEE Big Data

Conference Host: Ecole Technologie Superiere

ISSN: 2165-9605

ISBN: 978-3-901882-85-2

Record 339 of 491

Title: High-speed Regular Expression Matching with Pipelined Automata

Author(s): Matousek, D (Matousek, Denis); Korenek, J (Korenek, Jan); Pus, V (Pus, Viktor)

Edited by: Song YC; Wang S; Nelson B; Li J; Peng Y

Source: 2016 INTERNATIONAL CONFERENCE ON FIELD-PROGRAMMABLE TECHNOLOGY (FPT) **Pages:** 93-100 **Published:** 2016

Abstract: Pattern matching is a complex task which is widely used in network security monitoring applications. With the growing speed of network links, pattern matching architectures have to be improved in order to retain wire-speed processing. Multi-striding is a well-known technique on how to increase throughput of pattern matching architectures. In the paper we provide an analysis of scalability of multi-striding and show that it does not scale well and cannot be used for 100 Gbps throughput because utilization of FPGA resources grows exponentially. Therefore, we have designed a new hardware architecture for high-speed pattern matching that combines the multi-striding technique and parallel processing using pipelined finite state machines (FSMs). The architecture shares a single packet buffer for all parallel FSMs. Efficient implementation of the packet buffer reduces the number of BlockRAMs to 18% when compared to simple parallel implementation. Instead of multiplexing input data, the architecture pipelines the states of FSMs. Such pipelined processing with only local communication has a direct positive impact on frequency and throughput and allows us to scale the architecture to hundreds of Gbps.

Accession Number: WOS:000402988900012

Conference Title: 15th International Conference on Field-Programmable Technology (FPT)

Conference Date: DEC 07-09, 2016

Conference Location: Xian, PEOPLES R CHINA

Conference Sponsors: Harbin Ins Technol, Xian Jiaotong Univ, IEEE, IEEE Xian Sect, IEEE Harbin Sect, Xilinx, Intel, Natl Instruments, Synopsys

ISBN: 978-1-5090-5602-6

Record 340 of 491

Title: Experimental Validation of a Discrete Tire Model

Author(s): Jonak, M (Jonak, M.); Kasparek, J (Kasparek, J.); Kotek, L (Kotek, L.)

Book Group Author(s): Kaunas Univ Technol

Source: PROCEEDINGS OF THE 20TH INTERNATIONAL SCIENTIFIC CONFERENCE TRANSPORT MEANS 2016 **Book Series:** Transport Means - Proceedings of the International Conference **Pages:** 741-744 **Published:** 2016

Abstract: The article deals with the identification of input parameters and experimental validation of an off-road tire computational model. The model has been developed to solve contact tasks between wheel and soil. Computational model is based on a discrete element method. Experimental validation was performed by using a tired wheel TS-02 5.00-12 of VARI system. To identify input parameters, series of tasks were performed in order to measure dynamic behavior of the tire. Measurements were carried out in laboratory environment using a high-speed camera.

Accession Number: WOS:000402539900141

Conference Title: 20th International Scientific Conference on Transport Means

Conference Date: OCT 05-07, 2016

Conference Location: Juodkrante, LITHUANIA

Conference Sponsors: Kaunas Univ Technol, Klaipeda Univ, JSC Lithuanian Railways, IFToMM Natl Comm Lithuania, Lithuanian Soc Automot Engineers, Lithuanian Acad Sci, Div Tech Sci, Vilnius Gediminas Tech Univ

ISSN: 1822-296X

Record 341 of 491

Title: Design and Verification of a Large Combustion Chamber for Testing of Fuel Injection Nozzles

Author(s): Kotek, L (Kotek, L.); Jonak, M (Jonak, M.); Pistek, V (Pistek, V.); Drapal, L (Drapal, L.); Travnicek, P (Travnicek, P.)

Book Group Author(s): Kaunas Univ Technol

Source: PROCEEDINGS OF THE 20TH INTERNATIONAL SCIENTIFIC CONFERENCE TRANSPORT MEANS 2016 **Book Series:** Transport Means - Proceedings of the International Conference **Pages:** 997-1000 **Published:** 2016

Abstract: This article is focused on the design of a large combustion chamber for optical testing of nozzles of heavy-duty diesel engines with high-speed camera. This chamber must be optimized both in terms of optical parameters (uniformity of lightening, light flux), and in terms of safety (prevention of ignition of diesel fuel inside the chamber).

Accession Number: WOS:000402539900191

Conference Title: 20th International Scientific Conference on Transport Means

Conference Date: OCT 05-07, 2016

Conference Location: Juodkrante, LITHUANIA

Conference Sponsors: Kaunas Univ Technol, Klaipeda Univ, JSC Lithuanian Railways, IFToMM Natl Comm Lithuania, Lithuanian Soc Automot Engineers, Lithuanian Acad Sci, Div Tech Sci, Vilnius Gediminas Tech Univ

ISSN: 1822-296X

Record 342 of 491

Title: Passive NAT Detection Using HTTP Access Logs

Author(s): Komarek, T (Komarek, Tomas); Grill, M (Grill, Martin); Pevny, T (Pevny, Tomas)

Book Group Author(s): IEEE

Source: 2016 8TH IEEE INTERNATIONAL WORKSHOP ON INFORMATION FORENSICS AND SECURITY (WIFS 2016) **Book Series:** IEEE International Workshop on Information Forensics and Security **Published:** 2016

Abstract: Network devices performing Network Address Translation (NAT) overcome the problem of the deficit of IPv4 addresses as well as introduce a vulnerability to the network with possibly insecure configurations. Therefore detection of unauthorized NAT devices is an important task in the network security domain. In this paper, a novel passive NAT detection algorithm is proposed that identifies NAT devices in the network using statistical behavior analysis. We model behavior of network hosts using eight features extracted from HTTP access logs. These features are collected within consecutive non-overlapping time windows covering last 24 hours. To classify whether a host is a NAT device or an end host (non-NAT device) a pre-trained linear classifier is used. Since labeled data for training purposes is hard to obtain, we also propose a way how to generate the training data from unlabeled traffic logs. On the basis of our experimental evaluation, the detection algorithm outperforms the state-of-theart solution represented by [3].

Accession Number: WOS:000402749000006

Conference Title: 8th IEEE International Workshop on Information Forensics and Security (WIFS)

Conference Date: DEC 04-07, 2016

Conference Location: NYU Abu Dhabi, Abu Dhabi, U ARAB EMIRATES

Conference Sponsors: Ctr Cyber Secur, IEEE, IEEE Signal Proc Soc, IEEE Biometr Council, IEEE IFS

Conference Host: NYU Abu Dhabi

ISSN: 2157-4766

ISBN: 978-1-5090-1138-4

Record 343 of 491

Title: Reducing Cold Start Problems in Educational Recommender Systems

Author(s): Kuznetsov, S (Kuznetsov, Stanislav); Kordik, P (Kordik, Pavel); Rehorek, T (Rehorek, Tomas); Dvorak, J (Dvorak, Josef); Kroha, P (Kroha, Petr)

Book Group Author(s): IEEE

Source: 2016 INTERNATIONAL JOINT CONFERENCE ON NEURAL NETWORKS (IJCNN) **Book Series:** IEEE International Joint Conference on Neural Networks (IJCNN) **Pages:** 3143-3149 **Published:** 2016

Abstract: Educational data can help us to personalise university information systems. In this paper, we show how educational data can be used to improve the performance of interaction-based recommender systems. Educational data is transformed to student profiles helping to prevent cold start problems when recommending projects to students with few user interactions. Our results show that our hybrid interaction based recommender boosted by educational profiles significantly outperforms best-seller recommendation, which is a mainstream recommendation method for cold start users.

Accession Number: WOS:000399925503047

Conference Title: International Joint Conference on Neural Networks (IJCNN)

Conference Date: JUL 24-29, 2016

Conference Location: Vancouver, CANADA

Conference Sponsors: IEEE, IEEE Computat Intelligence Soc, Int Nueral Network Soc, Evolutionary Programming Soc, IET, IEEE BigData, Gulf Univ Sci & Technol

ISSN: 2161-4393

ISBN: 978-1-5090-0619-9

Record 344 of 491

Title: Evolution of multiple gaits for modular robots

Author(s): Vonasek, V (Vonasek, Vojtech); Faigl, J (Faigl, Jan)

Book Group Author(s): IEEE

Source: PROCEEDINGS OF 2016 IEEE SYMPOSIUM SERIES ON COMPUTATIONAL INTELLIGENCE (SSCI) **Published:** 2016

Abstract: Modular robots are composed of many elementary mechatronic modules that can be connected to form a robot body of various shapes. This feature allows such a robot to adapt for a given task and particular environment. A motion of the modular robot is based on control of individual angles between the modules, and the robot locomotion can be realized using Central Pattern Generators (CPG). A robot motion in the environment with obstacles can be achieved using several locomotion controllers that are switched by a strategy based on motion planning techniques. Preparation of CPG-based gaits leads to a high-dimensional optimization that requires to design proper cost functions. Existing approaches optimize the gaits separately according to human-designed cost functions. In this paper, we investigate how to automatically derive a set of gaits suitable for modular robots without specifying low-level details about the gaits. We propose to optimize multiple gaits simultaneously using a single cost function. This cost function is based on the ability of motion planning to solve the task using the gaits being optimized. The proposed system is verified on several modular robots with unusual shapes including robots with failed modules.

Accession Number: WOS:000400488302088

Conference Title: IEEE Symposium Series on Computational Intelligence (IEEE SSCI)

Conference Date: DEC 06-09, 2016

Conference Location: Athens, GREECE

Conference Sponsors: IEEE

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Faigl, Jan	E-8685-2013	0000-0002-6193-0792

ISBN: 978-1-5090-4240-1

Record 345 of 491

Title: A Novel and Efficient Method to Initialize FPGA Embedded Memory Content in Asymptotically Constant Time

Author(s): Bartik, M (Bartik, Matej); Ubik, S (Ubik, Sven); Kubalik, P (Kubalik, Pavel)

Edited by: Athanas P; Cumplido R; Feregrino C; Sass R

Source: 2016 INTERNATIONAL CONFERENCE ON RECONFIGURABLE COMPUTING AND FPGAS (RECONFIG16) **Book Series:** Proceedings International Conference on Reconfigurable Computing and FPGAs **Published:** 2016

Abstract: This paper describes analysis and implementation of a new method for maintaining valid content of FPGA memory blocks with an asymptotically constant time synchronous clear ability, that can be useful for (re) initialization to one default value. A particular application can be for high-speed real-time LZ77 [1] lossless compression algorithms, where a dictionary has to be (re) initialized before each run of the implemented compression algorithm.
The method is based on two most widely used techniques for clearing the memory content: a linear passage of the memory and clearing each cell by writing a default value and creating a register field providing an (in) valid bit for each memory cell. Our solution combines these two techniques together with the use of FPGA distributed memory blocks implemented in LUTs (Look-Up Tables) to overcome negative features of each previous method without losing the most of positive features. Our solution provides a balance between the two previous techniques and exceeds them in speed, resources utilization and latency of (re) initialization.

Accession Number: WOS:000400775800004

Conference Title: International Conference on Reconfigurable Computing and FPGAs (ReConFig)

Conference Date: NOV 30-DEC 02, 2016

Conference Location: Cancun, MEXICO

Conference Sponsors: Natl Inst Astrophys Opt & Elect Mexico, Virginia Tech, Univ N Carolina Charlotte, IEEE Circuits & Syst Soc, XILINX

ISSN: 2325-6532

ISBN: 978-1-5090-3707-0

Record 346 of 491

Title: Using Bayesian Modeling on Molecular Fragments Features for Virtual Screening

Author(s): Hoksza, D (Hoksza, David); Skoda, P (Skoda, Petr)

Book Group Author(s): IEEE

Source: 2016 IEEE CONFERENCE ON COMPUTATIONAL INTELLIGENCE IN BIOINFORMATICS AND COMPUTATIONAL BIOLOGY (CIBCB) **Published:** 2016

Abstract: Virtual screening enables to search large small-molecule compound libraries for active molecules with respect to given macromolecular target. In ligand-based virtual screening, this goal is achieved by utilizing information about fragments or patterns present in existing known active compounds. Typically, the patterns are encoded as fingerprints which are used to screen a database of candidate compounds. In this work, we introduce an approach which uses Bayesian inference to encode activity-related information. Unlike previous approaches, our method does not utilize simple fragments, but rather uses features of these fragments. For each molecule, we generate a set of molecular fragments and extract molecular features for each of them. Next, we remove correlated features and use the remaining ones to build a Bayes model of activity. To score a previously unseen molecule, the molecule's fragment feature vectors are passed to the model and a score is obtained as the aggregation of their probability scores. When screening a database, this score is used to rank the compounds database. We show on datasets with various levels of difficulty that using fragments features rather then fragments themselves results in improvement of retrieval rates with respect to the best state-of-the art molecular fingerprints.

Accession Number: WOS:000399465100018

Conference Title: 13th IEEE Annual Conference on Computational Intelligence in Bioinformatics and Computational Biology (IEEE CIBCB)

Conference Date: OCT 05-07, 2016

Conference Location: Chiang Mai, THAILAND

Conference Sponsors: IEEE, IEEE Computat Intelligence Soc, Thailand Convent & Exhibit Bur

ISBN: 978-1-4673-9472-7

Record 347 of 491

Title: Noncovalent Interactions by QMC: Speedup by One-Particle Basis-Set Size Reduction

Author(s): Dubecky, M (Dubecky, Matus)

Edited by: Tanaka S; Roy PN; Mitas L

Source: RECENT PROGRESS IN QUANTUM MONTE CARLO **Book Series:** ACS Symposium Series **Volume:** 1234 **Pages:** 119-126 **Published:** 2016

Abstract: While it is empirically accepted that the fixed-node diffusion Monte-Carlo (FN-DMC) depends only weakly on the size (beyond a certain reasonable level) of the one-particle basis sets used to expand its guiding functions, limits of this observation are not settled yet. Our recent work indicates that under the FN error cancellation conditions, augmented triple zeta basis sets are sufficient to achieve high-quality benchmark single-point energy differences in a number of small noncovalent complexes. In this preliminary progress report, we report on a possibility of significant truncation of the one-particle basis sets used to express the FN-DMC guiding functions, that has no visible effect on the accuracy of the production energy differences. The proposed scheme shows only modest increase of the local energy variance, indicating that the total CPU cost of large-scale benchmark noncovalent interaction energy FN-DMC calculations employing Gaussians may be reduced.

Accession Number: WOS:000399060600008

Conference Title: International Chemical Congress of Pacific-Basin-Societies

Conference Date: DEC 15-20, 2015

Conference Location: Honolulu, HI

Conference Sponsors: Amer Chem Soc, Div Chem Educ

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dubecky, Matus	P-1720-2016	

ISSN: 0097-6156

ISBN: 978-0-8412-3179-5

Record 348 of 491

Title: Simulation of UV/vis spectra of CyMe4BTBP and some of its degradation products

Author(s): Koubsky, T (Koubsky, Tomas); Schmidt, H (Schmidt, Holger); Modolo, G (Modolo, Giuseppe); Kalvoda, L (Kalvoda, Ladislav)

Edited by: Poinssot C; Bourg S

Source: ATALANTE 2016 INTERNATIONAL CONFERENCE ON NUCLEAR CHEMISTRY FOR SUSTAINABLE FUEL CYCLES **Book Series:** Procedia Chemistry **Volume:** 21 **Pages:** 509-516 **DOI:** 10.1016/j.proche.2016.10.071 **Published:** 2016

Abstract: Wet extraction and selective separation methods of actinide elements from highly active spent nuclear fuel constitutes a key step in the current waste reprocessing technologies. The quadridentate 6,6'-bis(1,2,4-triazin-3-y1)-2,2'-bipyridine ligands (BTBPs) form a very promising group of extraction agents investigated at recent. Radiation decay process of one of the BTBPs representatives, CyMe4BTBP, is indirectly analyzed by simulating the UV-Visible absorption spectra of the original compound and one proposed possible CyMe4BTBP and 1-octanol adduct and comparing the obtained courses with experimentally observed data. Ab-initio TDDFT approach using 6-31++G(d,p) basis set and wB97X, CAM-B3LYP, LC-wPBE functionals is applied. Partial agreement of the simulated and experimental data is found and discussed. (C) 201 6 The Authors. Published by Elsevier H.V.

Accession Number: WOS:000398055500071

Conference Title: 5th International ATALANTE International Conference on Nuclear Chemistry for Sustainable Fuel Cycles

Conference Date: JUN 05-10, 2016

Conference Location: Montpellier, FRANCE

Conference Sponsors: ATALANTE

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Modolo, Giuseppe		0000-0001-6490-5595
Schmidt, Holger		0000-0002-3448-3579

ISSN: 1876-6196

Record 349 of 491

Title: EVALUATION OF VARIOUS SPECTRAL INPUTS FOR ESTIMATION OF FOREST BIOCHEMICAL AND STRUCTURAL PROPERTIES FROM AIRBORNE IMAGING SPECTROSCOPY DATA

Author(s): Homolova, L (Homolova, L.); Janoutova, R (Janoutova, R.); Malenovsky, Z (Malenovsky, Z.)

Edited by: Halounova L; Sunar F; Potuckova M; Patkova L; Yoshimura M; Soergel U; BenDor E; Smit J; Bareth G; Zhang J; Kaasalainen S; Sorgel U; Osmanoglu B; Crespi M; Crosetto M; Blaschke T; Brovelli MA; Zagajewski B

Source: XXIII ISPRS CONGRESS, COMMISSION VII **Book Series:** International Archives of the Photogrammetry Remote Sensing and Spatial Information Sciences **Volume:** 41 **Issue:** B7 **Pages:** 961-966 **DOI:** 10.5194/isprsarchives-XLI-B7-961-2016 **Published:** 2016

Abstract: In this study we evaluated various spectral inputs for retrieval of forest chlorophyll content (Cab) and leaf area index (LAI) from high spectral and spatial resolution airborne imaging spectroscopy data collected for two forest study sites in the Czech Republic (beech forest at Stitna nad Vlari and spruce forest at BilV Kriz). The retrieval algorithm was based on a machine learning method - support vector regression (SVR). Performance of the four spectral inputs used to train SVR was evaluated: a) all available hyperspectral bands, b) continuum removal (CR) 645 - 710 nm, c) CR 705 - 780 nm, and d) CR 680 - 800 nm. Spectral inputs and corresponding SVR models were first assessed at the level of spectral databases simulated by combined leaf-canopy radiative transfer models PROSPECT and DART. At this stage, SVR models using all spectral inputs provided good performance (RMSE for Cab < 10 mu g cm(-2) and for LAI < 1.5), with consistently better performance for beech over spruce site. Since application of trained SVRs on airborne hyperspectral images of the spruce site produced unacceptably overestimated values, only the beech site results were analysed. The best performance for the Cab estimation was found for CR bands in range of 645 - 710 nm, whereas CR bands in range of 680 - 800 nm were the most suitable for LAI retrieval. The CR transformation reduced the across-track bidirectional reflectance effect present in airborne images due to large sensor field of view.

Accession Number: WOS:000393155900149

Conference Title: 23rd Congress of the International-Society-for-Photogrammetry-and-Remote-Sensing (ISPRS)

Conference Date: JUL 12-19, 2016

Conference Location: Prague, CZECH REPUBLIC

Conference Sponsors: Int Soc Photogrammetry & Remote Sensing

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Homolova, Lucie	A-8436-2011	
Janoutova, Ruzena	G-2755-2014	

ISSN: 2194-9034

Record 350 of 491

Title: Template-based prediction of RNA tertiary structure

Author(s): Galvanek, R (Galvanek, Rastislav); Hoksza, D (Hoksza, David); Panek, J (Panek, Josef)

Edited by: Tian T; Jiang Q; Liu Y; Burrage K; Song J; Wang Y; Hu X; Morishita S; Zhu Q; Wang G

Source: 2016 IEEE INTERNATIONAL CONFERENCE ON BIOINFORMATICS AND BIOMEDICINE (BIBM) **Book Series:** IEEE International Conference on Bioinformatics and Biomedicine-BIBM **Pages:** 1897-1900 **Published:** 2016

Abstract: RNA tertiary structure prediction approaches can be divided into two groups: de novo methods and template-based modeling. De novo are applicable only for small molecules while in case of medium and large size RNA molecules, template-based modeling needs to be employed. While this type of modeling is quite common in protein structure prediction field, there exist only very few tools for template-based RNA structure prediction. Therefore, we present a methodology for prediction of RNA three dimensional structure (target) utilizing a known structure of a related RNA molecule (template). First, the target and template sequences are aligned. Next, sequentially similar regions in the alignment are identified and corresponding substructures are transferred from template to target. The remaining parts of the target structures are predicted using an external tool. This phase includes treatment of indels and valid linking of the transferred and predicted portions of the target structure. Our proposed method is able to predict even large ribosomal RNA structures when sufficiently similar template is available. The experiments have shown that the main impact on the quality of prediction has the sequence similarity of the template and target and number of indels. For structures with size of hundreds of nucleotides with sequence similarity with template over 50% and ratio of indels up to 50% the method is able to generate target structures up to ten RMSD with respect to the reference structure.

Accession Number: WOS:000393191700323

Conference Title: IEEE International Conference on Bioinformatics and Biomedicine (IEEE BIBM)

Conference Date: DEC 15-18, 2016

Conference Location: Shenzhen, PEOPLES R CHINA

Conference Sponsors: IEEE, IEEE Comp Soc, Natl Sci Fdn, Harbin Inst Technol

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Galvanek, Rastislav	O-9974-2017	0000-0003-2844-6808

ISSN: 2156-1125

ISBN: 978-1-5090-1610-5

Close

Web of Science
Page 8 (Records 351 -- 400)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 351 of 491

Title: GENERATION OF ARABIDOPSIS LINES WITH ALTERED CYTOKININ LEVEL EXPRESSING GFP-FUSED CYTOSKELETAL PROTEINS

Author(s): Skalakova, P (Skalakova, Patricie); Fialova, V (Fialova, Vera)

Edited by: Polak O; Cerkal R; Belcredi NB; Horky P; Vacek P

Source: PROCEEDINGS OF INTERNATIONAL PHD STUDENTS CONFERENCE, (MENDELNET 2016) **Pages:** 757-762 **Published:** 2016

Abstract: Cell division, expansion and differentiation require a sophisticated spatial arrangement of the cytoskeleton. The ever increasing progress in fluorescent microscope techniques has allowed to visualize rearrangements and dynamics of actin and microtubule arrays in various cell types and tissues in plants. Processes controlling proper cytoskeleton organisation and its response to various stimuli, mediated by actin and microtubule binding proteins as well as plant hormones, are being an area of active investigation. As the current research of cytoskeleton regulation focused mainly on hormone auxin, the involvement of cytokinin is still unclear. In this study, we describe generation of transgenic lines of Arabidopsis thaliana comprising inducible system for manipulation of endogenous cytokinin level and simultaneously GFP-labelled actin or microtubule proteins. These lines serve as a tool for the study of cytokinin mode of action in the course of cell/organ development. Based on our results, it is obvious that cytokinins play a considerable role in modulation of plant cytoskeleton. However, further research is necessary to elucidate precise cytokinin signalling pathways and cross-talk with other hormones, which participate in such complex processes of cell morphology.

Accession Number: WOS:000392968500135

Conference Title: 23rd International PhD Students Conference (MendelNet)

Conference Date: NOV 09-10, 2016

Conference Location: Mendel Univ Brno, Fac AgriSciences, Brno, CZECH REPUBLIC

Conference Host: Mendel Univ Brno, Fac AgriSciences

ISBN: 978-80-7509-443-8

Record 352 of 491

Title: Concept Of An Effective Sentinel-1 Satellite SAR Interferometry System

Author(s): Lazecky, M (Lazecky, Milan); Comut, FC (Comut, Fatma Canaslan); Bakon, M (Bakon, Matus); Qin, Y (Qin, Yuxiao); Perissin, D (Perissin, Daniele); Hatton, E (Hatton, Emma); Spaans, K (Spaans, Karsten); Mendez, PJG (Mendez, Pablo J. Gonzalez); Guimaraes, P (Guimaraes, Pedro); de Sousa, JJM (de Sousa, Joaquim J. M.); Kocich, D (Kocich, David); Ustun, A (Ustun, Aydin)

Edited by: Varajao JEQ; CruzCunha MM; Martinho R; Rijo R; BjornAndersen N; Turner R; Alves D

Source: INTERNATIONAL CONFERENCE ON ENTERPRISE INFORMATION SYSTEMS/INTERNATIONAL CONFERENCE ON PROJECT MANAGEMENT/INTERNATIONAL CONFERENCE ON HEALTH AND SOCIAL CARE INFORMATION SYSTEMS AND TECHNOLOGIES, CENTERIS/PROJMAN / HCIST 2016 **Book Series:** Procedia Computer Science **Volume:** 100 **Pages:** 14-18 **DOI:** 10.1016/j.procs.2016.09.118 **Published:** 2016

Abstract: This brief study introduces a partially working concept being developed at IT4Innovations supercomputer (HPC) facility. This concept consists of several modules that form a whole body of an efficient system for observation of terrain or objects displacements using satellite SAR interferometry (InSAR). A metadata database helps to locate data stored in various storages and to perform basic analyzes. A special database has been designed to describe Sentinel-1 data, on its burst level. Custom Sentinel-1 TOPS processing algorithms allow an injection of coregistered bursts into the database. Once the area of interest is set and basic processing parameters are given, the selected data are merged and processed by the Persistent Scatterers (PS) InSAR method or an optimized Small Baselines (SB) InSAR derivative. Depending on the expected deliverables, the processing results can be post-analyzed using a custom approach, in order to achieve a set of reliable measurement points. Final results can be post processed and visualized using a custom GIS toolbox, consisting in open-source GIS functionality. The GIS post-processing is enforced by HPC power as well. To demonstrate the practical applicability of the described system, a subsidence area in Konya city, Turkey is used as the study area for Sentinel-1 InSAR evaluation. (C) 2016 The Authors. Published by Elsevier B.V.

Accession Number: WOS:000392695900002

Conference Title: International Conference on ENTERprise Information Systems / International Conference on Project MANagement / International Conference on Health and Social Care Information Systems and Technologies (CENTERIS/ProjMAN/HCist)

Conference Date: OCT 05-07, 2016

Conference Location: Porto, PORTUGAL

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ustun, Aydin	B-3427-2013	
Bakon, Matus		0000-0002-8850-9738
Sousa, Joaquim Joao		0000-0003-4533-930X
Lazecky, Milan		0000-0001-8179-5949

ISSN: 1877-0509

Record 353 of 491

Title: Brachythecium funkii Schimp. and B. japygum (Glow.) Kockinger & Jan Kucera comb. nov., two Alpine species hitherto included in B. cirrosum (Schwagr.) Schimp.

Author(s): Kockinger, H (Kockinger, Heribert); Kucera, J (Kucera, Jan)

Source: JOURNAL OF BRYOLOGY **Volume:** 38 **Issue:** 4 **Pages:** 267-285 **DOI:** 10.1080/03736687.2016.1156355 **Published:** 2016

Abstract: Morphological and molecular studies support the recognition of three alpine species within the traditional concept of Brachythecium cirrosum, which requires the resurrection of two earlier described taxa, B. funkii and B. japygum, comb. nov., from synonymy. According to nuclear and chloroplast sequence data, the latter two taxa proved to be closely related to B. tommasinii and B. tenuicaule, whereas the affinities of B. cirrosum within Brachythecium are rather unclear. B. funkii is a coarser plant than B. cirrosum and also differs in shorter leaf acumens and much larger lamina cells. On the other hand, B. japygum (better known under the illegitimate name Eurhynchium histrio) can be distinguished from B. cirrosum in the prostrate and densely pinnate to subdendroid growth form, longer leaf acumens and wider lamina cells with lumens wider than walls. All three species also differ from each other in the morphology of the alar cell group. Despite their shared preference for calcareous rocks, the three species show marked differences in habitat requirements.

Accession Number: WOS:000392918500001

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kucera, Jan	B-3633-2009	0000-0002-0230-5997

ISSN: 0373-6687

eISSN: 1743-2820

Record 354 of 491

Title: Complex manoeuvres of heterogeneous MAV-UGV formations using a model predictive control

Author(s): Spurny, V (Spurny, Vojtech); Baca, T (Baca, Tomas); Saska, M (Saska, Martin)

Book Group Author(s): IEEE

Source: 2016 21ST INTERNATIONAL CONFERENCE ON METHODS AND MODELS IN AUTOMATION AND ROBOTICS (MMAR) **Pages:** 998-1003 **Published:** 2016

Abstract: A problem of motion planning and coordination of compact formations of ground and aerial robots will be tackled in this paper. The scenarios when the formation composed from Unmanned Ground Vehicles (UGVs) and Unmanned Aerial Vehicles (UAVs), in particular Micro Aerial Vehicles (MAVs), has to reverse the direction of movement to fulfil task of collision-free motion to a target zone will be solved. The presented motion planning and stabilization approach provides an effective technique to enable deployment of closely cooperating teams of robots in outdoor as well as indoor environment. The formation to target region problem is solved using a Model Predictive Control (MPC) methodology and the formation driving concept is based on a virtual-leader-follower approach. The mentioned MPC based process is used for trajectory planning and control of a virtual leader and also for control and stabilization of followers (MAVs and UGVs). The proposed approach is verified with numerous simulations and hardware experiments.

Accession Number: WOS:000392500900175

Conference Title: 21st International Conference on Methods and Models in Automation and Robotics (MMAR)

Conference Date: AUG 29-SEP 01, 2016
Conference Location: Miedzyzdroje, POLAND
ISBN: 978-1-5090-1866-6

Record 355 of 491

Title: Application of Sampling-based Path Planning for Tunnel Detection in Dynamic Protein Structures
Author(s): Vonasek, V (Vonasek, Vojtech); Kozlikova, B (Kozlikova, Barbora)
Book Group Author(s): IEEE
Source: 2016 21ST INTERNATIONAL CONFERENCE ON METHODS AND MODELS IN AUTOMATION AND ROBOTICS (MMAR) **Pages:** 1010-1015 **Published:** 2016
Abstract: Behavior and properties of proteins as well as other bio-macromolecules is influenced by internal void space such as tunnels or cavities. Tunnels are paths leading from an active site inside the protein to its surface. Knowledge about tunnels and their evolution in time provides an insight into protein properties (e.g. stability or resistance to a co-solvent). Tunnels can be found using Voronoi diagrams (VD). To consider protein dynamics, that is represented by a sequence of protein snapshots, correspondences between VD in these snapshots need to be found. The computation of these correspondences is however time and memory consuming. In this paper, we propose a novel method for tunnel detection in dynamic proteins based on Rapidly Exploring Random Tree (RRT). The method builds a single configuration tree describing free space of the protein. The nodes of the tree are pruned according to protein dynamics. The proposed approach is compared to CAVER 3.0, one of the widely used freely available tools for protein analysis.
Accession Number: WOS:000392500900177
Conference Title: 21st International Conference on Methods and Models in Automation and Robotics (MMAR)
Conference Date: AUG 29-SEP 01, 2016
Conference Location: Miedzyzdroje, POLAND
ISBN: 978-1-5090-1866-6

Record 356 of 491

Title: Coexistence of Access and Backbone Networks with Sensor Systems
Author(s): Munster, P (Munster, Petr); Vojtech, J (Vojtech, Josef); Horvath, T (Horvath, Tomas); Havlis, O (Havlis, Ondrej); Slapak, M (Slapak, Martin); Skoda, P (Skoda, Pavel); Radil, J (Radil, Jan); Hula, M (Hula, Miloslav); Velc, R (Velc, Radek)
Book Group Author(s): IEEE
Source: 2016 INTERNATIONAL WORKSHOP ON FIBER OPTICS IN ACCESS NETWORK (FOAN) **Book Series:** International Workshop on Fiber Optics in Access Network **Published:** 2016
Abstract: In recent years, new applications as distributed fiber-optic sensing or precise time transfer have been widely studied and developed. Especially, with the growing interest for smart cities sensor networks have been developed intensively. Currently, individual optical fibers are mostly used for individual applications which is very inefficient and uneconomical, especially for longer distances. Moreover, construction of new routes for individual applications is often impossible. It is therefore necessary to use either dark fibers or sharing of a single fiber for multiple applications. Whereas the most of current and newly built access networks are based on optical fiber it is possible to find optical fiber almost everywhere - in city centers, along roads, etc. And since a usable bandwidth of a standard single mode optical fiber is sufficiently large it is appropriate to consider the possibility of coexistence. We performed simulations and experimental measurements to analyze requirements of individual applications and to confirm suitability of coexistence of sensor systems and 1.25 Gbps data transmission in a single optical fiber.
Accession Number: WOS:000392263400002
Conference Title: International Workshop on Fiber Optics in Access Network (FOAN)
Conference Date: OCT 18-19, 2016
Conference Location: Lisbon, PORTUGAL
ISSN: 2378-8488
ISBN: 978-1-5090-3319-5

Record 357 of 491

Title: Deep Neural Networks for Web Page Information Extraction
Author(s): Gogar, T (Gogar, Tomas); Hubacek, O (Hubacek, Ondrej); Sedivy, J (Sedivy, Jan)
Edited by: Iliadis L; Maglogiannis I
Source: ARTIFICIAL INTELLIGENCE APPLICATIONS AND INNOVATIONS, AIAI 2016 **Book Series:** IFIP Advances in Information and Communication Technology **Volume:** 475 **Pages:** 154-163 **DOI:** 10.1007/978-3-319-44944-9_14 **Published:** 2016
Abstract: Web wrappers are systems for extracting structured information from web pages. Currently, wrappers need to be adapted to a particular website template before they can start the extraction process. In this work we present a new method, which uses convolutional neural networks to learn a wrapper that can extract information from previously unseen templates. Therefore, this wrapper does not need any site-specific initialization and is able to extract information from a single web page. We also propose a method for spatial text encoding, which allows us to encode visual and textual content of a web page into a single neural net. The first experiments with product information extraction showed very promising results and suggest that this approach can lead to a general site-independent web wrapper.
Accession Number: WOS:000392413700014
Conference Title: 12th IFIP WG 12.5 International Conference on Artificial Intelligence Applications and Innovations (AIAI)
Conference Date: SEP 16-18, 2016
Conference Location: Thessaloniki, GREECE
Conference Sponsors: Int Federat Informat Proc Working Grp 12 5
ISSN: 1868-4238
ISBN: 978-3-319-44944-9; 978-3-319-44943-2

Record 358 of 491

Title: Avalanche Effect in Improperly Initialized CAESAR Candidates
Author(s): Ukrop, M (Ukrop, Martin); Svenda, P (Svenda, Petr)
Source: ELECTRONIC PROCEEDINGS IN THEORETICAL COMPUTER SCIENCE **Issue:** 233 **Pages:** 72-81 **DOI:** 10.4204/EPTCS.233.7 **Published:** 2016
Abstract: Cryptoprimitives rely on thorough theoretical background, but often lack basic usability features making them prone to unintentional misuse by developers. We argue that this is true even for the state-of-the-art designs. Analyzing 52 candidates of the current CAESAR competition has shown none of them have an avalanche effect in authentication tag strong enough to work properly when partially misconfigured. Although not directly decreasing their security profile, this hints at their security usability being less than perfect.
Accession Number: WOS:000390333200008
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Svenda, Petr	M-7619-2017	0000-0002-9784-7624

ISSN: 2075-2180

Record 359 of 491

Title: Dipolar molecules inside C-70: an electric field-driven room-temperature single-molecule switch
Author(s): Foroutan-Nejad, C (Foroutan-Nejad, Cina); Andrushchenko, V (Andrushchenko, Valery); Straka, M (Straka, Michal)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 48 **Pages:** 32673-32677 **DOI:** 10.1039/c6cp06986j **Published:** 2016
Abstract: We propose a two-state electric field-driven room-temperature single-molecule switch based on a dipolar molecule enclosed inside ellipsoidal fullerene C-70. We show that the two low-energy minima of the molecular dipole inside the C-70 cage provide distinguishable molecular states of the system that can be switched by application of an external electric field.
Accession Number: WOS:000390435800006
PubMed ID: 27892557
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Straka, Michal	E-5246-2011	0000-0002-7857-4990
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Andrushchenko, Valery		0000-0002-4874-0548

ISSN: 1463-9076
eISSN: 1463-9084

Record 360 of 491

Title: Shell shape and genetic variability of Southeast Asian Box Turtles (Cuora amboinensis) from Borneo and Sumatra
Author(s): Protiva, T (Protiva, Tomas); Gunalen, D (Gunalen, Danny); Bauerova, A (Bauerova, Anna); Palupcikova, K (Palupcikova, Klara); Somerova, B (Somerova, Barbora); Frydlova, P (Frydlova, Petra); Jancuchova-Laskova, J (Jancuchova-Laskova, Jitka); Simkova, O (Simkova, Olga); Frynta, D (Frynta, Daniel); Rehak, I (Rehak, Ivan)
Source: VERTEBRATE ZOOLOGY **Volume:** 66 **Issue:** 3 **Pages:** 387-396 **Published:** 2016
Abstract: Distinguishing between species is an essential aspect of animal research and conservation. For turtles, morphology and genetic analysis are potentially valuable tools for identification. Shell shape is an important component of phenotypic variation in turtles and can be easily described and quantified by geometric morphometrics (GM). Here, we focus on carapace and plastron shape discrimination of immature Southeast Asian box turtles (Cuora amboinensis) from two of the Greater Sunda Islands with partially distinct faunas. GM analysis identified significant differences in carapace and plastron shape between turtles from Borneo and Sumatra. The discrimination success amounted to 90% and 83.7% for carapace and plastron, respectively. The correlations of carapace and plastron shapes were high for Sumatra (0.846), and less pronounced for Borneo (0.560). We detected no differences in the ontogenetic trajectories of the shell shape between the two islands. We conclude that shell shape can be used for reliable geographic assignment of C. amboinensis of unknown origin. In addition to the comparison of shell shapes, turtles from Borneo, Sumatra, Seram, and turtles of unknown origin from two Czech zoos were studied genetically. Analysis of the complete mitochondrial cytochrome b gene confirmed the distinctness of turtles from Borneo and Sumatra, with p-distance 2.68 - 4.09% sequence difference. Moreover, we discovered considerable genetic difference in Seram turtles of previously unknown haplogroup (p-distance 6.00 - 8.68%) revealing the need for the revision of the whole species complex of Cuora amboinensis.
Accession Number: WOS:000389767200006
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Frydlova, Petra	P-5008-2016	0000-0001-9385-9743
Bauerova, Anna	D-6032-2014	0000-0001-9627-1945
Frynta, Daniel	L-7350-2016	0000-0002-1375-7972

ISSN: 1864-5755

Record 361 of 491

Title: Lipid molecules can induce an opening of membrane-facing tunnels in cytochrome P450 1A2
Author(s): Jerabek, P (Jerabek, Petr); Florian, J (Florian, Jan); Martinek, V (Martinek, Vaclav)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 44 **Pages:** 30344-30356 **DOI:** 10.1039/c6cp03692a **Published:** 2016
Abstract: Cytochrome P450 1A2 (P450 1A2, CYP1A2) is a membrane-bound enzyme that oxidizes a broad range of hydrophobic substrates. The structure and dynamics of both the catalytic and trans-membrane (TM) domains of this enzyme in the membrane/water environment were investigated using a multiscale computational approach, including coarse-grained and all-atom molecular dynamics. Starting from the spontaneous self-assembly of the system containing the TM or soluble domain immersed in randomized dilauroyl phosphatidylcholine (DLPC)/water mixture into their respective membrane-bound forms, we reconstituted the membrane-bound structure of the full-length P450 1A2. This structure includes a TM helix that spans the membrane, while being connected to the catalytic domain by a short flexible loop. Furthermore, in this model, the upper part of the TM helix interacts directly with a conserved and highly hydrophobic N-terminal proline-rich segment of the catalytic domain; this segment and the FG loop are immersed in the membrane, whereas the remaining portion of the catalytic domain remains exposed to aqueous solution. The shallow membrane immersion of the catalytic domain induces a depression in the opposite intact layer of the phospholipids. This structural effect may help in stabilizing the position of the TM helix directly beneath the catalytic domain. The partial immersion of the catalytic domain also allows for the enzyme substrates to enter the active site from either aqueous solution or phospholipid environment via several solvent-and membrane-facing tunnels in the full-length P450 1A2. The calculated tunnel dynamics indicated that the opening probability of the membrane-facing tunnels is significantly enhanced when a DLPC molecule spontaneously penetrates into the membrane-facing tunnel 2d. The energetics of the lipid penetration process were assessed by the linear interaction energy (LIE) approximation, and found to be thermodynamically feasible.
Accession Number: WOS:000388492900014
PubMed ID: 27722524
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Martinek, Vaclav	E-6710-2011	0000-0003-3321-4526
Jerabek, Petr	A-1223-2013	0000-0002-5175-6890
Florian, Jan	E-1554-2012	0000-0003-2669-4293

ISSN: 1463-9076
eISSN: 1463-9084

Record 362 of 491

Title: Solvent effects on ion-receptor interactions in the presence of an external electric field
Author(s): Novak, M (Novak, Martin); Foroutan-Nejad, C (Foroutan-Nejad, Cina); Marek, R (Marek, Radek)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 18 **Issue:** 44 **Pages:** 30754-30760 **DOI:** 10.1039/c6cp05781k **Published:** 2016
Abstract: In this work we investigated the influence of an external electric field on the arrangement of the solvent shells around ions interacting with a carbon-based receptor. Our survey reveals that the mechanism of interaction between a monoatomic ion and a pi-type ion receptor varies by the variation in the solvent polarity, the nature of the ion, and the strength of the external field. The characteristics of the ion-surface interaction in nonpolar solvents are similar to those observed in a vacuum. However, in water, we identified two mechanisms. Soft and polarizable ions preferentially interact with the p-receptor. In contrast, two bonded states were found for hard ions. A fully solvated ion, weakly interacting with the receptor at weak field, and a strong p-complex at the strong-field regime were identified. An abrupt variation in the potential energy surface (PES) associated with the rearrangement of the solvation shell on the surface of the receptor induced by an external field was observed both in implicit and explicit solvent environments. The electric field at which the solvation shell breaks is proportional to the hardness of the ion as has been suggested recently based on experimental observations.
Accession Number: WOS:000388492900056
PubMed ID: 27796379
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Novak, Martin	I-3248-2015	0000-0001-5067-1994
Marek, Radek	D-6929-2012	0000-0002-3668-3523

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eISSN: 1463-9084

Record 363 of 491

Title: Effect of lead and caesium on the mechanical, vibrational and thermodynamic properties of hexagonal fluorocarbonates: a comparative first principles study
Author(s): Rao, EN (Rao, E. Narsimha); Vaitheeswaran, G (Vaitheeswaran, G.); Reshak, AH (Reshak, A. H.); Auluck, S (Auluck, S.)
Source: RSC ADVANCES **Volume:** 6 **Issue:** 102 **Pages:** 99885-99897 **DOI:** 10.1039/c6ra20408b **Published:** 2016

Abstract: Exploration of the structure-property correlation of fluorocarbon materials has received much interest over recent years due to their extremely strong nonlinear optical (NLO) responses (13.6 times that of KH2PO4(KDP)), good ultraviolet (UV) cutoff (<200 nm) with better mechanical and chemical stability. In the present work a novel CsPbCO3F, ABCO(3)F (A = K, Rb; B = Ca, Sr) series is explored using density functional theory (DFT) calculations focusing on their mechanical, vibrational and thermodynamic properties and their Born effective charge (BEC) tensors. The calculated structural properties of lead carbonate fluoride with a semi-empirical dispersion corrected Ortmann Bechstedt Schmidt (OBS) method are found to be in relatively close agreement with experimental data. The obtained single crystal elastic constants satisfy the Born's mechanical stability criteria. The calculated bulk modulus value of lead carbonate (41 GPa) indicates its soft nature compared with other studied carbonates and is observed to be harder than KDP (26 GPa). In addition we have calculated the polycrystalline properties, bulk modulus (B), shear modulus (G), Young's modulus (E) and Poisson's ratio (sigma) of CsPbCO3F and ABCO3F (A = K, Rb; B = Ca, Sr) using the Voigt, Reuss and Hill approximations. The obtained B/G (>1.75) results reveal the ductile nature of all the studied materials except for KCaCO3F (1.67) which is found to be brittle. Results of the hexagonal shear anisotropic factors (A(1), A(2), A(3)) indicate that all the studied crystals possess considerable mechanical anisotropy. Calculated zone centered vibrational infrared (IR) spectra confirm the higher optical activity of CsPbCO3F compared with the other carbonates. The obtained high frequency modes are consistent with the experimental values. The obtained BECs reveal the presence of a mixed covalent-ionic character of the compounds. The thermodynamic properties, namely entropy, Debye temperature, heat capacity, enthalpy, thermal expansion and thermal conductivity, have been computed at different temperatures ranging from 5 K to 1000 K. The results show that the lead based compound has the highest thermal conductivity (32.430 W m(-1) K-1) of the reported carbonate materials. The results clearly indicate that the material could show better durability than LiNbO3, alpha-SiO2, CaCO3, and Ba3B6O12 hexagonal NLO materials. All the computed thermodynamic properties indicate that CsPbCO3F might be a potential candidate for second-order NLO applications. The polycrystalline, vibrational and thermodynamic properties of carbonate materials presented in this work could be a step forward in the process of developing new NLO materials.

Accession Number: WOS:000386439800033

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363

ISSN: 2046-2069

Record 364 of 491

Title: The Great Recession in the Non-EMU Visegrad Countries: A Nonlinear DSGE Model with Time-Varying Parameters

Author(s): Tvrz, S (Tvrz, Stanislav); Vasicek, O (Vasicek, Osvald)

Source: FINANCE A UVER-CZECH JOURNAL OF ECONOMICS AND FINANCE **Volume:** 66 **Issue:** 3 **Pages:** 207-235 **Published:** 2016

Abstract: Inspired by the radically different course and aftermath of the Great Recession in the Polish economy and the economies of the Czech Republic and Hungary in contrast to their comparable economic development before the crisis, we investigate the structural stability of these three Central European economies in that period. The question of structural stability is essential for proper application of a standard DSGE model in a given economy. In the case of significant structural changes, these should be incorporated explicitly into the model structure in order to avoid misleading results. Each of the three economies is represented by a nonlinear small open economy dynamic stochastic general equilibrium model with a financial accelerator. First, the DSGE models are estimated using Bayesian methods under the assumption of constant structural parameters. Then the development of time-varying structural parameters is estimated by means of a particle filter using second order approximation of a nonlinear DSGE model. We find several statistically significant structural changes in the Czech and Polish economies. According to the time-varying impulse response functions, the structural changes during the Great Recession curbed the negative impacts of the adverse exogenous shocks to a certain extent in the Czech and Polish economies. By contrast, the vulnerability of the Hungarian economy further increased.

Accession Number: WOS:000384820200002

ISSN: 0015-1920

Record 365 of 491

Title: Electrocatalytic monitoring of peptidic proton-wires

Author(s): Dorcak, V (Dorcak, V.); Kabelac, M (Kabelac, M.); Kroutil, O (Kroutil, O.); Bednarova, K (Bednarova, K.); Vacek, J (Vacek, J.)

Source: ANALYST **Volume:** 141 **Issue:** 15 **Pages:** 4554-4557 **DOI:** 10.1039/c6an00869k **Published:** 2016

Abstract: The transfer of protons or proton donor/acceptor abilities is an important phenomenon in many biomolecular systems. One example is the recently proposed peptidic proton-wires (H-wires), but the ability of these His-containing peptides to transfer protons has only been studied at the theoretical level so far. Here, for the first time the proton transfer ability of peptidic H-wires is examined experimentally in an adsorbed state using an approach based on a label-free electrocatalytic reaction. The experimental findings are complemented by theoretical calculations at the ab initio level in a vacuum and in an implicit solvent. Experimental and theoretical results indicated Ala(3)(His-Ala(2))(6) to be a high proton-affinity peptidic H-wire model. The methodology presented here could be used for the further investigation of the proton-exchange chemistry of other biologically or technologically important macromolecules.

Accession Number: WOS:000381426100003

PubMed ID: 27353221

ISSN: 0003-2654

eISSN: 1364-5528

Record 366 of 491

Title: Revealing the spin-polarized optical properties of monoclinic alpha-Eu-2(MoO4)(3): a DFT + U approach

Author(s): Reshak, AH (Reshak, A. H.)

Source: RSC ADVANCES **Volume:** 6 **Issue:** 57 **Pages:** 51675-51682 **DOI:** 10.1039/c6ra06022f **Published:** 2016

Abstract: The spin polarized complex first-order linear optical dispersion reveals the spin-polarized electronic structure of alpha-Eu-2(MoO4)(3). Calculation explored the influence of the generalized gradient approximation plus the Hubbard Hamiltonian (GGA + U) on the band dispersion and the energy band gap of the spin-up and spin-down and hence on the optical transitions. The appearance of Eu-4f states on the conduction band minimum of the spin-up case causes a significant influence on the ground state properties of alpha-Eu-2(MoO4)(3). The calculated optical properties reveal that alpha-Eu-2(MoO4)(3) possesses an indirect energy gap of about 2.2 eV (up arrow) and 3.2 eV (down arrow) in close agreement with the measured one (3.74 eV). The all-electron full potential linear augmented plane wave (FPLAPW + lo) method within GGA + U was used. We have applied U on the 4f orbitals of Eu atoms and 4d orbitals of Mo atoms to correct the ground state. We have taken a careful look at the valence band's electronic charge density distribution to visualize the charge transfer and the chemical bonding characteristics. The optical properties were calculated seeking deep insight into the electronic structure. It has been found that alpha-Eu-2(MoO4)(3) exhibits positive uniaxial anisotropy and negative birefringence for spin-up and spin-down configurations.

Accession Number: WOS:000382079800024

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363

ISSN: 2046-2069

Record 367 of 491

Title: DFT combined to Boltzmann transport theory for optoelectronic and thermoelectric properties investigations for monoclinic metallic selenide: Cu5Sn2Se7

Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Goumri-Said, S (Goumri-Said, Souraya)

Source: OPTIK **Volume:** 127 **Issue:** 13 **Pages:** 5472-5478 **DOI:** 10.1016/j.ijleo.2016.02.073 **Published:** 2016

Abstract: We combined a density functional theory (DFT) and Boltzmann transport theory to investigate the optoelectronic and thermoelectric properties of the monoclinic selenide Cu5Sn2Se7 compound. The present selenide is found metallic and has shown similarities with the recent selenides based on transition metals. The Fermi level is surrounded by the Cu-d, Sn-s and Se-p states along with the small contribution of Cu-s/p, Sn-p/d and Se-d states. The investigated optical properties illustrated that the major transitions take place from Cu-d and Se-p states below E-F to the Sn-s states above E-F. DFT calculations were combined to Boltzmann transport theory to extract the thermoelectric properties depending on temperature such as the resistivity, thermal and electrical conductivity, Seebeck coefficient and figure of merit (ZT). Our theoretical thermoelectric properties show a very close agreement with available experimental data.

Accession Number: WOS:000376810000057

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Azam, Sikander		0000-0001-5923-1127

ISSN: 0030-4026

Record 368 of 491

Title: The surface stability and equilibrium crystal morphology of Ni2P nanoparticles and nanowires from an ab initio atomistic thermodynamic approach

Author(s): He, JJ (He, Junjie); Morales-Garcia, A (Morales-Garcia, Angel); Bludsky, O (Bludsky, Ota); Nachtigall, P (Nachtigall, Petr)

Source: CRYSTENGCOMM **Volume:** 18 **Issue:** 21 **Pages:** 3808-3818 **DOI:** 10.1039/c6ce00584e **Published:** 2016

Abstract: Knowledge of the equilibrium crystal shape and structure of the exposed surfaces of nickel phosphide (Ni2P) nanostructures is essential for understanding and control of their catalytic performance. Ab initio atomistic thermodynamics was used to investigate computationally the effects of the experimental conditions (temperature, pressure, and chemical potentials) on the relative stabilities of low-Miller index surfaces and on the equilibrium crystal morphology of Ni2P nanoparticles and nanowires. The P-covered (0001)-Ni3P2 (denoted as (0001)-A-P) surface was found to be the most stable surface at a considerably wide range of chemical potentials, whereas the (0001)-A, (10 (1) over bar1)-Ni/P and (10 (1) over bar2)-Ni/P surfaces are the thermodynamically most favored phases just in narrow chemical potential regions. The theoretical equilibrium shapes and structures of the Ni2P nanoparticles and nanowires were obtained based on the Wulff construction at various chemical potentials. The morphology of the surfaces of the Ni2P nanoparticles and nanowires does depend on the chemical potential; thus, it can be tailored for particular applications by a suitable choice of experimental conditions. The (0001), (10 (1) over bar0) and (10 (1) over bar1) side facets dominate the nanoparticle surface in a wide range of chemical potentials but other side facets can also appear at particular ranges of chemical potentials. Results reported herein give new insight into the Ni2P nanoparticle morphology showing how it depends on the experimental conditions; this information can help to tailor the surface and shape of Ni2P nanoparticles for specific applications, e.g., in catalysis.

Accession Number: WOS:000377085700008

Author Identifiers:

Author	ResearcherID Number	ORCID Number
He, Junjie	O-6825-2017	0000-0001-6447-7893
Nachtigall, Petr	A-6220-2013	0000-0002-1628-7275
Bludsky, Ota	A-5659-2008	
Morales Garcia, Angel		0000-0003-0491-1234

ISSN: 1466-8033

Record 369 of 491

Title: Synthesis and characterization of carbosilane dendrimer-sodium montmorillonite clay nanocomposites. Experimental and theoretical studies

Author(s): Strasak, T (Strasak, Tomas); Maly, M (Maly, Marek); Mullerova, M (Mullerova, Monika); Cermak, J (Cermak, Jan); Kormunda, M (Kormunda, Martin); Capkova, P (Capkova, Pavla); Matousek, J (Matousek, Jindrich); Stastna, LC (Stastna, Lucie Cervenkova); Rejnek, J (Rejnek, Jaroslav); Holubova, J (Holubova, Jana); Jandova, V (Jandova, Vera); Cepe, K (Cepe, Klara)

Source: RSC ADVANCES **Volume:** 6 **Issue:** 49 **Pages:** 43356-43366 **DOI:** 10.1039/c6ra04442e **Published:** 2016

Abstract: Novel organic/inorganic hybrid materials with carbosilane fillers were developed. New carbosilane dendrimers of the first (Dm1) and second (Dm2) generations bearing four and eight cationic ammonium groups on their periphery were synthesized first. Their structure was elucidated by NMR spectroscopy and ESI-HRMS whereas their thermal stability was confirmed by TGA. Both dendrimers were used as organic components in the preparation of organoclays. A series of nanocomposites Dm1Mt and Dm2Mt with varied contents of dendrimers were prepared and characterized by a wide variety of analytical techniques. The analytical data show that the structure of organoclays and the ability of dendrimers to effectively interact with montmorillonite are strongly affected by their generation. Both species Dm1 and Dm2 intercalated into the interlayer space of montmorillonite increase correspondingly the basal spacing of Mt. In contrast to Dm2, increased loadings of Dm1 in suspension during the intercalation process have a negligible effect on d-spacing in the studied concentration range, as confirmed by XRD analysis. Besides unmodified Mt we also studied the interactions of dendrimers with plasma treated Mt and the results are presented. Computer modelling based mainly on Molecular Dynamics has shown the non-linear dependence of the d-spacing on the amount of dendrimers in the interlayer space within the studied dendrimer/montmorillonite mass ratio interval. The filling capacity of plasma unmodified montmorillonite with respect to both dendrimers was estimated using a combination of experimental and theoretical results.

Accession Number: WOS:000375611100069

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Maly, Marek	H-5757-2015	0000-0002-5930-563X
Cermak, Jan	H-3475-2014	
Mullerova, Monika	N-6966-2017	0000-0002-2505-5230
Strasak, Tomas	H-3493-2014	0000-0001-6413-0494
Cervenkova Stastna, Lucie	H-3476-2014	
Kormunda, Martin	M-2990-2013	

ISSN: 2046-2069

Record 370 of 491

Title: Intense chirality induction in nitrile solvents by a helquat dye monitored by near resonance Raman scattering

Author(s): Sebestik, J (Sebestik, Jaroslav); Teply, F (Teply, Filip); Cisarova, I (Cisarova, Ivana); Vavra, J (Vavra, Jan); Koval, D (Koval, Dusan); Bour, P (Bour, Petr)

Source: CHEMICAL COMMUNICATIONS **Volume:** 52 **Issue:** 37 **Pages:** 6257-6260 **DOI:** 10.1039/c6cc01606e **Published:** 2016

Abstract: Chirality induction phenomena attract attention because of their relevance to intermolecular interactions encountered in living matter. Usually, such effects are weak. However, enantiomers of a [6]helquat dye were found to induce exceptionally strong chirality in several achiral solvents containing nitrile groups. This effect was observable as an intense Raman optical activity (ROA) induced in acetonitrile, acetonitrile-d(3), and liquid hydrogen cyanide solvents. The observation was verified by measurement of both helquat enantiomers which provided mirror image ROA spectra. Theoretical analysis indicated that the 532 nm laser excitation light was in a near resonance with electronic transitions of the dye, which made the effect observable in very dilute solutions (1 : 200000 helquat to nitrile ratio) and thus the phenomenon can be generally useful in analytical chemistry.

Accession Number: WOS:000375620400010

PubMed ID: 27087537

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sebestik, Jaroslav	C-9166-2012	0000-0002-0614-2064
Cisarova, Ivana	B-1385-2017	0000-0002-9612-9831
Koval, Dusan	G-5432-2014	0000-0002-6424-3891
Teply, Filip		0000-0003-3459-556X

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Record 371 of 491

Title: Mean squared displacement from fluorescence correlation spectroscopy

Author(s): Kubecka, J (Kubecka, Jakub); Uhlik, F (Uhlik, Filip); Kosovan, P (Kosovan, Peter)

Source: SOFT MATTER **Volume:** 12 **Issue:** 16 **Pages:** 3760-3769 **DOI:** 10.1039/c6sm00296j **Published:** 2016

Abstract: Under certain conditions, the mean squared displacement (MSD) can be retrieved from fluorescence correlation spectroscopy (FCS) measurements. However, in the general case this procedure is not valid, and the apparent MSD obtained from FCS data may substantially differ from the true one. In this work we discuss under which conditions this procedure can be applied. Furthermore, we use computer simulations to obtain the MSD and the apparent MSD for the diffusion of a single polymer chain under various approximations. Based on the simulation results we discuss the reliability of the apparent MSD obtained from FCS, showing that it systematically deviates from the true MSD. We also propose a general procedure to verify the reliability of the apparent MSD by measurements at various focal spot sizes.

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PubMed ID: 26996953

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kubecka, Jakub	M-6245-2017	0000-0002-8002-0911
Kosovan, Peter	A-1945-2008	0000-0002-6708-3344
Uhlik, Filip	G-7395-2012	0000-0002-1628-2861

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Record 372 of 491

Title: Phylogenetic position of Geitleribactron purpureum (Synechococcales, Cyanobacteria/Cyanophyceae) and its implications for the taxonomy of Chamaesiphonaceae and Leptolyngbyaceae

Author(s): Mares, J (Mares, Jan); Cantonati, M (Cantonati, Marco)

Source: FOTTEA **Volume:** 16 **Issue:** 1 **Pages:** 104-111 **DOI:** 10.5507/fot.2016.002 **Published:** 2016

Abstract: Over the last decades, the taxonomy of cyanobacteria has been considerably improved and restructured due to the increase in data output from molecular phylogeny. Recently, a new protocol was developed that enables reliable sequencing of 16S rRNA genes in cultivation-resistant cyanobacteria using analysis of single cells, filaments, or colonies. In the current study, we examined a sample of a heteropolar unicellular cyanobacterium, Geitleribactron purpureum, from the holotype material (deep epilithon of Lake Tovel, Western Dolomites, Italy). We isolated and purified single colonies of G. purpureum, and subjected them to direct PCR and 16S rRNA gene sequencing. We obtained a congruent set of sequences that formed a unique, isolated cyanobacterial lineage, showing phylogenetic clustering among simple filamentous genera of the family Leptolyngbyaceae. We provide evidence for deep polyphyly in Chamaesiphonaceae, and suggest that Geitleribactron should be re-classified in the Leptolyngbyaceae.

Accession Number: WOS:000373585200008

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cantonati, Marco	G-4278-2018	0000-0003-0179-3842
Mares, Jan	B-2395-2009	0000-0002-5745-7023

ISSN: 1802-5439

Record 373 of 491

Title: The structure and dynamics of chitin nanofibrils in an aqueous environment revealed by molecular dynamics simulations

Author(s): Strelcova, Z (Strelcova, Zora); Kulhanek, P (Kulhanek, Petr); Friak, M (Friak, Martin); Fabritius, HO (Fabritius, Helge-Otto); Petrov, M (Petrov, Michal); Neugebauer, J (Neugebauer, Joerg); Koca, J (Koca, Jaroslav)

Source: RSC ADVANCES **Volume:** 6 **Issue:** 36 **Pages:** 30710-30721 **DOI:** 10.1039/c6ra00107f **Published:** 2016

Abstract: Chitin is one of the most abundant structural biomolecules in nature, where it occurs in the form of nanofibrils that are the smallest building blocks for many biological structural materials, such as the exoskeleton of Arthropoda. Despite this fact, little is known about the structural properties of these nanofibrils. Here, we present a theoretical study of a single chitin molecule and 10 alpha-chitin nanofibrils with different numbers of chains in an aqueous environment that mimics the conditions in natural systems during self-assembly. Our extensive analysis of the molecular dynamics trajectories, including free energy calculations for every model system, reveals not only the structural properties of the nanofibrils, but also provides insight into the principles of nanofibril formation. We identified the fundamental phenomena occurring in the chitin nanofibrils such as their hydrogen bonding pattern and resulting helical shape. With increasing size, the nanofibrils become increasingly stable and their structural properties approach those of crystalline alpha-chitin if they consist of more than 20 chains. Interestingly, this coincides with the typical size of chitin nanofibrils observed in natural systems, suggesting that their evolutionary success was at least partially driven by these specific structure-property relations.

Accession Number: WOS:000373061600093

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kulhanek, Petr	D-6884-2012	0000-0002-4152-6514
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Petrov, Michal	R-8723-2017	0000-0002-8680-6317

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Record 374 of 491

Title: Phylogeny and population genetic structure of the ant genus Acropyga (Hymenoptera : Formicidae) in Papua New Guinea

Author(s): Janda, M (Janda, Milan); Matos-Maravi, P (Matos-Maravi, Pavel); Borovanska, M (Borovanska, Michaela); Zima, J (Zima, Jan, Jr.); Youngerman, E (Youngerman, Eric); Pierce, NE (Pierce, Naomi E.)

Source: INVERTEBRATE SYSTEMATICS **Volume:** 30 **Issue:** 1 **Pages:** 28-40 **DOI:** 10.1071/IS14050 **Published:** 2016

Abstract: Spatial isolation and geological history are important factors in the diversification and population differentiation of species. Here we describe distributional patterns of ants in the genus Acropyga across Papua New Guinea (PNG), a highly biodiverse but little-studied region. We estimate phylogenetic relationships among currently recognised species of Acropyga and assess population genetic structure of the widespread species, A. acutiventris, across lowland areas of the island. We find that species of Acropyga present in PNG diversified during the Pliocene, between six and two million years ago. Most species now exhibit a patchy distribution that does not show a strong signal of geological history. However, the population genetic structure of the widespread species A. acutiventris has been influenced by geography, habitat association and, possibly, historical habitat fragmentation. There is a significant effect of isolation-by-distance within continuous lowland forest, and proximity to Australia has had a larger impact in structuring populations of A. acutiventris in PNG than has the Central Papuan Cordillera. This study is the first to describe population genetic patterns of an ant species in Papua New Guinea.

Accession Number: WOS:000372805500002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Matos-Maravi, Pavel	O-6626-2017	0000-0002-2885-4919
Borovanska, Michaela	D-1263-2016	
Janda, Milan	H-7216-2014	

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Record 375 of 491

Title: Microsatellite analysis of four similar Euphrasia (Orobanchaceae) species changes the traditional view of this group

Author(s): Svobodova, S (Svobodova, Sarka); Kosnar, J (Kosnar, Jiri); Koutecky, P (Koutecky, Petr); Stech, M (Stech, Milan)

Source: PLANT ECOLOGY AND EVOLUTION **Volume:** 149 **Issue:** 1 **Pages:** 45-58 **DOI:** 10.5091/plecevo.2016.1128 **Published:** 2016

Abstract: Background and aims-The genus Euphrasia comprises a taxonomically intricate group. In Central Europe, E. nemorosa and E. stricta are widely accepted species. However, the occurrence of putative intermediate morphotypes considered to be the result of regular hybridization makes identification of populations often difficult. Besides these mostly late-flowering species, two mostly early-flowering species, E. coerulea and E. slovaca, are distinguished in the Sudeten and in the Carpathians, respectively. Because of the doubtful nature of intermediate forms and difficult distinction of early-flowering morphotypes, the aims of this study were to find genetically supported groups and test morphological differences among them.

Methods and key results - We conducted a survey of the genetical and morphological diversity in 42 populations, which were assigned to four species based on morphology. Using microsatellite analysis, we discovered three genetic groups within our data set. Whereas E. stricta and E. nemorosa comprised separate clusters, most of the early-flowering populations identified as E. coerulea and E. slovaca formed one common cluster. Traditional characters such as corolla length, branching and the presence of a long awn on the bracts were identified in multivariate analyses as the most reliable morphological differences between genetically defined E. stricta and E. nemorosa. Early-flowering populations differed generally by their low number of nodes. In spite of their genetic similarity, they differed morphologically between the two geographical areas. In spite of the assumption of different selling rates correlated with corolla size, differences in genetic diversity among populations with different corolla sizes were not found.

Conclusions - There are three well supported groups in the studied dataset of Euphrasia species. Delimitation of E. stricta and E. nemorosa is in concert with traditional views, but

delimitation of the third group changes the traditional distinction of two mostly early-flowering species in the study area.
Accession Number: WOS:000371196200006
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koutecky, Petr	D-7284-2016	

ISSN: 2032-3913
eISSN: 2032-3921

Record 376 of 491
Title: Cyber performances, technical and artistic collaboration across continents
Author(s): Ubik, S (Ubik, Sven); Navratil, J (Navratil, Jiri); Melnikov, J (Melnikov, Jiri); Goo, B (Goo, Boncheol); Noor, FNM (Noor, Faridah Noor Mohd); Baumann, A (Baumann, Alain); Hrb, J (Hrb, Jaroslav); Allocchio, C (Allocchio, Claudio); Castillo, G (Castillo, Gerard)
Source: FUTURE GENERATION COMPUTER SYSTEMS-THE INTERNATIONAL JOURNAL OF ESCIENCE **Volume:** 54 **Pages:** 306-312 **DOI:** 10.1016/j.future.2015.06.009 **Published:** JAN 2016
Abstract: Our objective was to verify whether modern computer network and audiovisual technologies can enable collaborative work between performing artists when they are distributed across large distances and what the requirements and limitations are. Such distributed collaborative environments will bring new opportunities both for the artists and the audience.
We describe our experiences gained from laboratory experiments and during cyber performances at APAN meetings that took place in Korea and Taiwan. (c) 2015 Elsevier B.V. All rights reserved.
Accession Number: WOS:000368383200024
ISSN: 0167-739X
eISSN: 1872-7115

Record 377 of 491
Title: Toward natural multi-user interaction in advanced collaborative display environments
Author(s): Rusnak, V (Rusnak, Vit); Rucka, L (Rucka, Lukas); Holub, P (Holub, Petr)
Source: FUTURE GENERATION COMPUTER SYSTEMS-THE INTERNATIONAL JOURNAL OF ESCIENCE **Volume:** 54 **Pages:** 313-325 **DOI:** 10.1016/j.future.2015.03.019 **Published:** JAN 2016
Abstract: Large high-resolution displays have become widely spread in research centers, laboratories, and public spaces during the last decade. There have been various research efforts in transformation of these displays from passive screens to interactive environments where multiple users can interact independently with multi-touch surfaces, in-air interaction or pointing devices. Such systems provide basic multi-user interaction, i.e., two or more users can interact concurrently. However, continuous user tracking and association of input events with users, which could considerably improve user experience, is still a largely unexplored topic. In this paper, we present a set of techniques enabling cue-less multi-user interaction in environments where horizontal or vertical high-resolution displays are in the role of central visualization platforms. We define the concept of cue-less multi-user interaction and set of techniques that enable unobtrusive user tracking and their association with input events through combination of a multi-touch surface and a depth sensor. Further, we introduce an open-source framework implementing techniques behind this concept and their evaluation in terms of accuracy of user association and the overall system interactivity when integrated with selected distributed rendering middleware. (c) 2015 Elsevier B.V. All rights reserved.
Accession Number: WOS:000368383200025
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Rusnak, Vit		0000-0003-1493-2194
Holub, Petr		0000-0002-5358-616X

ISSN: 0167-739X
eISSN: 1872-7115

Record 378 of 491
Title: High-performance forward error correction: Enabling multi-gigabit flows and beyond on commodity GPU and CPU hardware in presence of packet loss
Author(s): Kabat, M (Kabat, Milan); David, V (David, Vojtech); Holub, P (Holub, Petr); Pulec, M (Pulec, Martin)
Source: FUTURE GENERATION COMPUTER SYSTEMS-THE INTERNATIONAL JOURNAL OF ESCIENCE **Volume:** 54 **Pages:** 326-335 **DOI:** 10.1016/j.future.2015.04.007 **Published:** JAN 2016
Abstract: In demanding real-time multimedia transmissions, even a small packet loss might significantly degrade the visual quality. As retransmission is not an option in real-time transfers especially when transmitting the data over long distances, it is necessary to employ mechanisms of Forward Error Correction (FEC). Low-Density Generator Matrix (LDGM) codes are known to be suitable for coding on large block sizes, however, high bitrates of currently used video formats (FullHD, 4K) also require high throughput of FEC coding and decoding. We propose a parallel design of LDGM encoding and decoding algorithms suitable for off-the-shelf, (massively) parallel platforms, such CPUs with vector units or GPUs, and evaluate our approach in real-world scenarios of high-definition and 4K video transmissions. Our results show that offloading FEC computation to such platform is beneficial for low-latency, high-quality multimedia transmissions and may even enable transmissions beyond 10Gbps once the commodity network interfaces reach this speed. (C) 2015 Elsevier B.V. All rights reserved.
Accession Number: WOS:000368383200026
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Holub, Petr		0000-0002-5358-616X

ISSN: 0167-739X
eISSN: 1872-7115

Record 379 of 491
Title: Fine tuning of graphene properties by modification with aryl halogens
Author(s): Bousa, D (Bousa, D.); Pumera, M (Pumera, M.); Sedmidubsky, D (Sedmidubsky, D.); Sturala, J (Sturala, J.); Luxa, J (Luxa, J.); Mazanek, V (Mazanek, V.); Sofer, Z (Sofer, Z.)
Source: NANOSCALE **Volume:** 8 **Issue:** 3 **Pages:** 1493-1502 **DOI:** 10.1039/c5nr06295k **Published:** 2016
Abstract: Graphene and its derivatives belong to one of the most intensively studied materials. The radical reaction using halogen derivatives of arene-diazonium salts can be used for effective control of graphene's electronic properties. In our work we investigated the influence of halogen atoms (fluorine, chlorine, bromine and iodine) as well as their position on the benzene ring towards the electronic and electrochemical properties of modified graphenes. The electronegativity as well as the position of the halogen atoms on the benzene ring has crucial influence on graphene's properties due to the inductive and mesomeric effects. The results of resistivity measurement are in good agreement with the theoretical calculations of electron density within chemically modified graphene sheets. Such simple chemical modifications of graphene can be used for controllable and scalable synthesis of graphene with tunable transport properties.
Accession Number: WOS:000368040200032
PubMed ID: 26676958
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bousa, Daniel	W-4902-2017	0000-0002-6228-7508
Sedmidubsky, David	K-3874-2015	0000-0003-3191-8781
Pumera, Martin	F-2724-2010	0000-0001-5846-2951
Sofer, Zdenek	A-9690-2010	0000-0002-1391-4448
Sturala, Jiri	G-8229-2017	0000-0002-8113-0709

ISSN: 2040-3364
eISSN: 2040-3372

Record 380 of 491

Title: Predictive control and stabilization of nonholonomic formations with integrated spline-path planning

Author(s): Saska, M (Saska, Martin); Spurny, V (Spurny, Vojtech); Vonasek, V (Vonasek, Vojtech)

Source: ROBOTICS AND AUTONOMOUS SYSTEMS **Volume:** 75 **Pages:** 379-397 **DOI:** 10.1016/j.robot.2015.09.004 **Part:** B **Published:** JAN 2016

Abstract: path planning in the space of multinominals integrated into a model predictive control mechanism for driving formations of autonomous mobile robots is presented in this paper. The proposed approach is designed to stabilize the formations in desired shapes, and to navigate the group into a final position in a partly known environment with dynamic obstacles. In addition, the system provides inter-vehicle coordination and collision avoidance in the event of failure of a team member. The method is aimed at reaching the final position of the formation in the desired shape, but it enables to change temporarily this shape if it is enforced by the environment (in narrow corridors, on response to an impending collision with obstacles and faulty team members, etc.). This autonomous emergent behaviour increases the robustness of the system and its usability. It enables a proper compromise to be found between the formation driving requirement and the effort to fulfil the mission objective, i.e., to move the group from the current state into the required position. In this paper, the convergence of the method and the requirements for stability are shown on the basis of the results of the Lyapunov theorems of stability. These theoretical achievements imply constraints on the applicability of the system, which are verified in numerical simulations and in various tests with real autonomous robots. The performances of the entire system and of independent sub-systems in various formation driving scenarios are also shown in these tests. (C) 2015 Elsevier B.V. All rights reserved.

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ISSN: 0921-8890
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Record 381 of 491

Title: Engel-Vosko GGA Approach Within DFT Investigations of the Optoelectronic Structure of the Metal Chalcogenide Semiconductor CsAgGa2Se4

Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Goumri-Said, S (Goumri-Said, Souraya)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 45 **Issue:** 1 **Pages:** 746-754 **DOI:** 10.1007/s11664-015-4192-8 **Published:** JAN 2016

Abstract: Metal chalcogenide semiconductors have a significant role in the development of materials for energy and nanotechnology applications. First principle calculations were applied on CsAgGa2Se4 to investigate its optoelectronic structure and bonding characteristics, using the full-potential linear augmented plane wave method within the framework of generalized gradient approximations (GGA) and Engel-Vosko GGA functionals (EV-GGA). The band structure from EV-GGA shows that the valence band maximum and conduction band minimum are situated at I" with a band gap value of 2.15 eV. A mixture of orbitals from Ag 4p (6)/4d (10), Se 3d (10), Ga 4p (1), Se 4p (4) , and Ga 4s (2) states have a primary role to lead to a semiconducting character of the present chalcogenide. The charge density iso-surface shows a strong covalent bonding between Ag-Se and Ga-Se atoms. The imaginary part of dielectric constant reveals that the threshold (first optical critical point) energy of dielectric function occurs 2.15 eV. It is obvious that with a direct large band gap and large absorption coefficient, CsAgGa2Se4 might be considered a potential material for photovoltaic applications.

Accession Number: WOS:000367467800089

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Azam, Sikander		0000-0001-5923-1127

ISSN: 0361-5235
eISSN: 1543-186X

Record 382 of 491

Title: Telomere binding protein TRB1 is associated with promoters of translation machinery genes in vivo

Author(s): Schrumpfova, PP (Schrumpfova, Petra Prochazkova); Vychodilova, I (Vychodilova, Ivona); Hapala, J (Hapala, Jan); Schorova, S (Schorova, Sarka); Dvoracek, V (Dvoracek, Vojtech); Fajkus, J (Fajkus, Jiri)

Source: PLANT MOLECULAR BIOLOGY **Volume:** 90 **Issue:** 1-2 **Pages:** 189-206 **DOI:** 10.1007/s11103-015-0409-8 **Published:** JAN 2016

Abstract: Recently we characterised TRB1, a protein from a single-myb-histone family, as a structural and functional component of telomeres in Arabidopsis thaliana. TRB proteins, besides their ability to bind specifically to telomeric DNA using their N-terminally positioned myb-like domain of the same type as in human shelterin proteins TRF1 or TRF2, also possess a histone-like domain which is involved in protein-protein interactions e.g., with POT1b. Here we set out to investigate the genome-wide localization pattern of TRB1 to reveal its preferential sites of binding to chromatin in vivo and its potential functional roles in the genome-wide context. Our results demonstrate that TRB1 is preferentially associated with promoter regions of genes involved in ribosome biogenesis, in addition to its roles at telomeres. This preference coincides with the frequent occurrence of telobox motifs in the upstream regions of genes in this category, but it is not restricted to the presence of a telobox. We conclude that TRB1 shows a specific genome-wide distribution pattern which suggests its role in regulation of genes involved in biogenesis of the translational machinery, in addition to its preferential telomeric localization.

Accession Number: WOS:000367345300014
PubMed ID: 26597966

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fajkus, Jiri	D-2499-2012	0000-0002-3112-1716
Hapala, Jan	K-4983-2012	0000-0003-0568-5806

ISSN: 0167-4412
eISSN: 1573-5028

Record 383 of 491

Title: Some Like it High! Phylogenetic Diversity of High-Elevation Cyanobacterial Community from Biological Soil Crusts of Western Himalaya

Author(s): Capkova, K (Capkova, Katerina); Hauer, T (Hauer, Tomas); Rehakova, K (Rehakova, Klara); Dolezal, J (Dolezal, Jiri)

Source: MICROBIAL ECOLOGY **Volume:** 71 **Issue:** 1 **Pages:** 113-123 **DOI:** 10.1007/s00248-015-0694-4 **Published:** JAN 2016

Abstract: The environment of high-altitudinal cold deserts of Western Himalaya is characterized by extensive development of biological soil crusts, with cyanobacteria as dominant component. The knowledge of their taxonomic composition and dependency on soil chemistry and elevation is still fragmentary. We studied the abundance and the phylogenetic diversity of the culturable cyanobacteria and eukaryotic microalgae in soil crusts along altitudinal gradients (4600-5900 m) at two sites in the dry mountains of Ladakh (SW Tibetan Plateau and Eastern Karakoram), using both microscopic and molecular approaches. The effects of environmental factors (altitude, mountain range, and soil physico-chemical parameters) on the composition and biovolume of phototrophs were tested by multivariate redundancy analysis and variance partitioning. Both phylogenetic diversity and composition of morphotypes were similar between Karakorum and Tibetan Plateau. Phylogenetic analysis of 16S rRNA gene revealed strains belonging to at least five genera. Besides clusters of common soil genera, e.g., Microcoleus, Nodosilinea, or Nostoc, two distinct clades of simple trichal taxa were newly discovered. The most abundant cyanobacterial orders were Oscillatoriales and Nostacales, whose biovolume increased with increasing elevation, while that of Chroococales decreased. Cyanobacterial species richness was low in that only 15 morphotypes were detected. The environmental factors accounted for 52 % of the total variability in microbial data, 38.7 % of which was explained solely by soil chemical properties, 14.5 % by altitude, and 8.4 % by mountain range. The elevation, soil phosphate, and magnesium were the most important predictors of soil phototrophic communities in both mountain ranges despite their different bedrocks and origin. The present investigation represents a first record on phylogenetic diversity of the cyanobacterial community of biological soil crusts from Western Himalayas and first record from altitudes over 5000 m.

Accession Number: WOS:000367097500012
PubMed ID: 26552394

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Capkova, Katerina	M-1430-2014	
Hauer, Tomas	F-5089-2010	0000-0002-8005-5874
Rehakova, Klara	B-2143-2012	

ISSN: 0095-3628

eISSN: 1432-184X

Record 384 of 491

Title: Metadyn View: Fast web-based viewer of free energy surfaces calculated by metadynamics

Author(s): Hosek, P (Hosek, Petr); Spiwok, V (Spiwok, Vojtech)

Source: COMPUTER PHYSICS COMMUNICATIONS **Volume:** 198 **Pages:** 222-229 **DOI:** 10.1016/j.cpc.2015.08.037 **Published:** JAN 2016

Abstract: Metadynamics is a highly successful enhanced sampling technique for simulation of molecular processes and prediction of their free energy surfaces. An in-depth analysis of data obtained by this method is as important as the simulation itself. Although there are several tools to compute free energy surfaces from metadynamics data, they usually lack user friendliness and a build-in visualization part. Here we introduce Metadyn View as a fast and user friendly viewer of bias potential/free energy surfaces calculated by metadynamics in Plumed package. It is based on modern web technologies including HTML5JavaScript and Cascade Style Sheets (CSS). It can be used by visiting the web site and uploading a HILLS file. It calculates the bias potential/free energy surface on the client-side, so it can run online or offline without necessity to install additional web engines. Moreover, it includes tools for measurement of free energies and free energy differences and data/image export.
Program summary
Program title: Metadyn View
Catalogue identifier: AEYC_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEYC_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: GPL v3.0
No. of lines in distributed program, including test data, etc.: 273269
No. of bytes in distributed program, including test data, etc.: 4632839
Distribution format: tar.gz
Programming language: HTML5, JavaScript, CSS, WebGL.
Computer: Any computer with a modern web browser compatible with HTML5, JavaScript and CSS.
Operating system: Platform-independent.
RAM: Depends on the number of Gaussian hills and dimensionality of the bias potential.
Classification: 3, 7.7, 23.
Nature of problem: Fast and interactive visualization of free energy surfaces of molecular systems calculated by metadynamics method.
Solution method: Implementation of optimized Bias Sum algorithm and a set of tools for free energy surface analysis.
Unusual features: The program, due to its web-based nature, can be run on a wide range of devices and without installation.
Running time: Couple of seconds for a medium sized HILLS file (tens of thousands of lines). (C) 2015 Elsevier B.V. All rights reserved.

Accession Number: WOS:000365370800020

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Spiwok, Vojtech	A-7747-2008	0000-0001-8108-2033

ISSN: 0010-4655
eISSN: 1879-2944

Record 385 of 491

Title: Force field for realistic molecular dynamics simulations of ZrO2 growth

Author(s): Houska, J (Houska, Jiri)

Source: COMPUTATIONAL MATERIALS SCIENCE **Volume:** 111 **Pages:** 209-217 **DOI:** 10.1016/j.commatsci.2015.09.025 **Published:** JAN 2016

Abstract: The paper primarily deals with the development of an interaction potential (force field) for a realistic description of atom-by-atom ZrO2 growth. Owing to the fact that for many metal oxides including ZrO2 only full-charge (Zr+4 and O-2) interaction potentials are available, special attention is paid to the effect of the Zr and O elemental charges. Parameters of the short-range part of the interaction potential leading to experimental lattice parameters and formation energies have been identified in a wide range of elemental charges. Molecular dynamics simulations of ZrO2 growth reveal that the structures grown using the presently available full-charge interaction potentials are in contradiction with an experiment (the atoms have too low coordination numbers). Simulations using a wide range of newly fitted full-charge and partial-charge interaction potentials reveal that the results depend (in addition to the fitting procedure) on the elemental charges. Correct partial charges and potential parameters leading to experimentally relevant structures (with correct coordination numbers) have been identified and used. (C) 2015 Elsevier B.V. All rights reserved.

Accession Number: WOS:000364164400029

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Houska, Jiri	B-9616-2016	0000-0002-4809-4128

ISSN: 0927-0256
eISSN: 1879-0801

Record 386 of 491

Title: Optimal conditions for opening of membrane pore by amphiphilic peptides

Author(s): Kabelka, I (Kabelka, Ivo); Vacha, R (Vacha, Robert)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 143 **Issue:** 24 **Article Number:** 243115 **DOI:** 10.1063/1.4933229 **Published:** DEC 28 2015

Abstract: Amphiphilic peptides can interact with biological membranes and severely affect their barrier and signaling functions. These peptides, including antimicrobial peptides, can self-assemble into transmembrane pores that cause cell death. Despite their medical importance, the conditions required for pore formation remain elusive. Monte Carlo simulations with coarse-grained models enabled us to calculate the free energies of pore opening under various conditions. In agreement with oriented circular dichroism experiments, a high peptide-to-lipid ratio was found to be necessary for spontaneous pore assembly. The peptide length has a non-monotonic impact on pore formation, and the optimal length matches with the membrane thickness. Furthermore, the hydrophobicity of the peptide ends and the mutual positions of peptides on the membrane play a role. (C) 2015 AIP Publishing LLC.

Accession Number: WOS:000370412900021
PubMed ID: 26723600
ISSN: 0021-9606
eISSN: 1089-7690

Record 387 of 491

Title: The drag of the tails: Diffusion of sticky nanoparticles in dilute polymer solutions

Author(s): Kuldova, J (Kuldova, Jitka); Uhlik, F (Uhlik, Filip); Kosovan, P (Kosovan, Peter)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 143 **Issue:** 24 **Article Number:** 243129 **DOI:** 10.1063/1.4935389 **Published:** DEC 28 2015

Abstract: We devise a simple coarse-grained model of a nanoparticle exhibiting attractive interactions with a polymer in good solvent and use Monte Carlo simulations to study how adsorption of the polymer affects the hydrodynamic properties of the nanoparticle. We show that the hydrodynamic radius of the polymer-decorated nanoparticle increases with increasing polymer chain length or concentration. The slowdown of diffusion of the sticky nanoparticles is predicted to occur at polymer concentrations many orders of magnitude below the overlap concentration, in contrast with the case of non-sticky nanoparticles. To rationalize our findings, we employ the concept of trains, loops, and tails, which has been used in earlier theoretical studies of polymer adsorption at interfaces. We show that dominant contribution to the increase of the hydrodynamic radius of the polymer-decorated nanoparticles comes from the tails, which stretch far from the surface. On the contrary, the much more numerous but shorter loops and tails play only a minor role. (C) 2015 AIP Publishing LLC.

Accession Number: WOS:000370412900035
PubMed ID: 26723614

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kosovan, Peter	A-1945-2008	0000-0002-6708-3344
Uhlik, Filip	G-7395-2012	0000-0002-1628-2861

ISSN: 0021-9606
eISSN: 1089-7690

Record 388 of 491

Title: Phylogenetic Reconstruction of the Calosphaeriales and Togniniales Using Five Genes and Predicted RNA Secondary Structures of ITS, and Flabellascus tenuirostris gen. et sp nov.

Author(s): Reblova, M (Reblova, Martina); Jaklitsch, WM (Jaklitsch, Walter M.); Reblova, K (Reblova, Kamila); Stepanek, V (Stepanek, Vaclav)

Source: PLOS ONE **Volume:** 10 **Issue:** 12 **Article Number:** e0144616 **DOI:** 10.1371/journal.pone.0144616 **Published:** DEC 23 2015

Abstract: The Calosphaeriales is revisited with new collection data, living cultures, morphological studies of ascoma centrum, secondary structures of the internal transcribed spacer (ITS) rDNA and phylogeny based on novel DNA sequences of five nuclear ribosomal and protein-coding loci. Morphological features, molecular evidence and information from predicted RNA secondary structures of ITS converged upon robust phylogenies of the Calosphaeriales and Togniniales. The current concept of the Calosphaeriales includes the Calosphaeriaceae and Pleurostomataceae encompassing five monophyletic genera, Calosphaeria, Flabellascus gen. nov., Jattaea, Pleurostoma and Togniniella, strongly supported by Bayesian and Maximum Likelihood methods. The structural elements of ITS1 form characteristic patterns that are phylogenetically conserved, corroborate observations based on morphology and have a high predictive value at the generic level. Three major clades containing 44 species of Phaeoacremonium were recovered in the closely related Togniniales based on ITS, actin and beta-tubulin sequences. They are newly characterized by sexual and RNA structural characters and ecology. This approach is a first step towards understanding of the molecular systematics of Phaeoacremonium and possibly its new classification. In the Calosphaeriales, Jattaea aphanospora sp. nov. and J. ribicola sp. nov. are introduced, Calosphaeria taediosa is combined in Jattaea and epitypified. The sexual morph of Phaeoacremonium cinereum was encountered for the first time on decaying wood and obtained in vitro. In order to achieve a single nomenclature, the genera of asexual morphs linked with the Calosphaeriales are transferred to synonymy of their sexual morphs following the principle of priority, i.e. Calosphaeriophora to Calosphaeria, Phaeocrella to Togniniella and Pleurostomophora to Pleurostoma. Three new combinations are proposed, i.e. Pleurostoma ochraceum comb. nov., P. repens comb. nov. and P. richardsiae comb. nov. The morphology-based key is provided to facilitate identification of genera accepted in the Calosphaeriales.

Accession Number: WOS:000367092600027
PubMed ID: 26699541
ISSN: 1932-6203

Record 389 of 491

Title: Non-Catalyzed Click Reactions of ADIBO Derivatives with 5-Methyluridine Azides and Conformational Study of the Resulting Triazoles

Author(s): Smyslova, P (Smyslova, Petra); Popa, I (Popa, Igor); Lycka, A (Lycka, Antonin); Tejral, G (Tejral, Gracian); Hlavac, J (Hlavac, Jan)

Source: PLOS ONE **Volume:** 10 **Issue:** 12 **Article Number:** e0144613 **DOI:** 10.1371/journal.pone.0144613 **Published:** DEC 16 2015

Abstract: Copper-free click reactions between a dibenzoazocine derivative and azides derived from 5-methyluridine were investigated. The non-catalyzed reaction yielded both regioisomers in an approximately equivalent ratio. The NMR spectra of each regioisomer revealed conformational isomery. The ratio of isomers was dependent on the type of regioisomer and the type of solvent. The synthesis of various analogs, a detailed NMR study and computational modeling provided evidence that the isomery was dependent on the interaction of the azocine and pyrimidine parts.

Accession Number: WOS:000366722700048
PubMed ID: 26673606
ISSN: 1932-6203

Record 390 of 491

Title: Molecular systematics of Barbatosphaeria (Sordariomycetes): multigene phylogeny and secondary ITS structure

Author(s): Reblova, M (Reblova, M.); Reblova, K (Reblova, K.); Stepanek, V (Stepanek, V.)

Source: PERSOONIA **Volume:** 35 **Pages:** 21-38 **DOI:** 10.3767/003158515X687434 **Published:** DEC 2015

Abstract: Thirteen morphologically similar strains of barbatosphaeria- and tectonidula-like fungi were studied based on the comparison of cultural and morphological features of sexual and asexual morphs and phylogenetic analyses of five nuclear loci, i.e. internal transcribed spacer rDNA operon (ITS), large and small subunit nuclear ribosomal DNA, beta-tubulin, and second largest subunit of RNA polymerase II. Phylogenetic results were supported by in-depth comparative analyses of common core secondary structure of ITS1 and ITS2 in all strains and the identification of non-conserved, co-evolving nucleotides that maintain base pairing in the RNA transcript. Barbatosphaeria is defined as a well-supported monophyletic clade comprising several lineages and is placed in the Sordariomycetes incertae sedis. The genus is expanded to encompass nine species with both septate and non-septate ascospores in clavate, stipitate asci with a non-amyloid apical annulus and non-stromatic ascomata with a long decumbent neck and carbonised wall often covered by pubescence. The asexual morphs are dematiaceous hyphomycetes with holoblastic conidiogenesis belonging to Ramichloridium and Sporothrix types. The morphologically similar Tectonidula, represented by the type species T. hippocrepida, grouped with members of Barbatosphaeria and is transferred to that genus. Four new species are introduced and three new combinations in Barbatosphaeria are proposed. A dichotomous key to species accepted in the genus is provided.

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PubMed ID: 26823626
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Stepanek, Vaclav	H-7456-2014	

ISSN: 0031-5850

Record 391 of 491

Title: Mesomeric Effects of Graphene Modified with Diazonium Salts: Substituent Type and Position Influence its Properties

Author(s): Bousa, D (Bousa, Daniel); Jankovsky, O (Jankovsky, Ondrej); Sedmidubsky, D (Sedmidubsky, David); Luxa, J (Luxa, Jan); Sturala, J (Sturala, Jiri); Pumera, M (Pumera, Martin); Sofer, Z (Sofer, Zdenek)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 21 **Issue:** 49 **Pages:** 17728-17738 **DOI:** 10.1002/chem.201502127 **Published:** DEC 1 2015

Abstract: In the last decade, graphene and graphene derivatives have become some of the most intensively studied materials. Tuning of the electronic and electrochemical properties of graphene is of paramount importance. In this study, six diazonium-modified graphenes containing different functional groups according to the diazonium salt precursor were investigated. These diazonium moieties have a strong mesomeric (resonance) effect and act as either electron-donating or -withdrawing species. Different graphene precursors, such as thermally and chemically reduced graphenes were studied. All the products were characterized in detail by elemental combustion analysis, FTIR spectroscopy, Raman spectroscopy, high-resolution X-ray photoelectron spectroscopy (XPS), and cyclic voltammetry. Resistivity and zeta potential measurements were consistent with theoretical (DFT) calculations. The results show that chemical modification of graphene by diazotation strongly influences its properties, creating a huge application potential in microelectronics, energy storage and conversion devices, and electrocatalysis.

Accession Number: WOS:000367185700028
PubMed ID: 26494288
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sofer, Zdenek	A-9690-2010	0000-0002-1391-4448
Sturala, Jiri	G-8229-2017	0000-0002-8113-0709
Sedmidubsky, David	K-3874-2015	0000-0003-3191-8781
Bousa, Daniel	W-4902-2017	0000-0002-6228-7508
Pumera, Martin	F-2724-2010	0000-0001-5846-2951

ISSN: 0947-6539
eISSN: 1521-3765

Record 392 of 491

Title: CER/TER - THE NEW METRIC FOR TCP CONNECTION ROBUSTNESS EVALUATION AND COMPARISON
Author(s): Vondrous, O (Vondrous, Ondrej); Macejko, P (Macejko, Peter); Kocur, Z (Kocur, Zbynek)
Source: ADVANCES IN ELECTRICAL AND ELECTRONIC ENGINEERING **Volume:** 13 **Issue:** 5 **Pages:** 522-528 **DOI:** 10.15598/aeee.v13i5.1500 **Published:** DEC 2015
Abstract: This article presents new metric for TCP connection robustness evaluation and comparison. This metric is focused on TCP connection and transmission continuity rather then on maximal throughput or minimal RTT. This metric is developed especially for evaluation of narrow band networks. That is why it is very convenient to use this metric for networks such as Internet of Things networks or industrial sensor networks. Our metric is based on observing if connections or transmissions are successfully finished or not. It is possible to optimize this metric for specific situations. This metric can be used in both the real networks and in discrete simulation environments.
Accession Number: WOS:000409460300016
ISSN: 1336-1376
eISSN: 1804-3119

Record 393 of 491
Title: In Depth Characterization of Repetitive DNA in 23 Plant Genomes Reveals Sources of Genome Size Variation in the Legume Tribe Fabeae
Author(s): Macas, J (Macas, Jiri); Novak, P (Novak, Petr); Pellicer, J (Pellicer, Jaume); Cizkova, J (Cizkova, Jana); Koblizkova, A (Koblizkova, Andrea); Neumann, P (Neumann, Pavel); Fukova, I (Fukova, Iva); Dolezel, J (Dolezel, Jaroslav); Kelly, LJ (Kelly, Laura J.); Leitch, IJ (Leitch, Ilia J.)
Source: PLOS ONE **Volume:** 10 **Issue:** 11 **Article Number:** e0143424 **DOI:** 10.1371/journal.pone.0143424 **Published:** NOV 25 2015
Abstract: The differential accumulation and elimination of repetitive DNA are key drivers of genome size variation in flowering plants, yet there have been few studies which have analysed how different types of repeats in related species contribute to genome size evolution within a phylogenetic context. This question is addressed here by conducting large-scale comparative analysis of repeats in 23 species from four genera of the monophyletic legume tribe Fabeae, representing a 7.6-fold variation in genome size. Phylogenetic analysis and genome size reconstruction revealed that this diversity arose from genome size expansions and contractions in different lineages during the evolution of Fabeae. Employing a combination of low-pass genome sequencing with novel bioinformatic approaches resulted in identification and quantification of repeats making up 55-83% of the investigated genomes. In turn, this enabled an analysis of how each major repeat type contributed to the genome size variation encountered. Differential accumulation of repetitive DNA was found to account for 85% of the genome size differences between the species, and most (57%) of this variation was found to be driven by a single lineage of Ty3/gypsy LTR-retrotransposons, the Ogre elements. Although the amounts of several other lineages of LTR-retrotransposons and the total amount of satellite DNA were also positively correlated with genome size, their contributions to genome size variation were much smaller (up to 6%). Repeat analysis within a phylogenetic framework also revealed profound differences in the extent of sequence conservation between different repeat types across Fabeae. In addition to these findings, the study has provided a proof of concept for the approach combining recent developments in sequencing and bioinformatics to perform comparative analyses of repetitive DNAs in a large number of non-model species without the need to assemble their genomes.
Accession Number: WOS:000365865300065
PubMed ID: 26606051
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fukova, Iva	G-9415-2014	0000-0002-2472-0665
Pellicer, Jaume	L-3048-2015	0000-0001-7632-9775
Macas, Jiri	G-8618-2014	0000-0003-0829-1570
Novak, Petr	A-3059-2013	0000-0002-5068-9681
Neumann, Pavel	H-7345-2013	0000-0001-6711-6639

ISSN: 1932-6203

Record 394 of 491
Title: Complete genome sequence of Clostridium pasteurianum NRRL B-598, a non-type strain producing butanol
Author(s): Sedlar, K (Sedlar, Karel); Kolek, J (Kolek, Jan); Skutkova, H (Skutkova, Helena); Branska, B (Branska, Barbora); Provaznik, I (Provaznik, Ivo); Patakova, P (Patakova, Petra)
Source: JOURNAL OF BIOTECHNOLOGY **Volume:** 214 **Pages:** 113-114 **DOI:** 10.1016/j.jbiotec.2015.09.022 **Published:** NOV 20 2015
Abstract: The strain Clostridium pasteurianurn NRRL B-598 is non-type, oxygen tolerant, spore-forming, mesophilic and heterofermentative strain with high hydrogen production and ability of acetone-butanol fermentation (ethanol production being negligible). Here, we present the annotated complete genome sequence of this bacterium, replacing the previous draft genome assembly. The genome consisting of a single circular 6,186,879 bp chromosome with no plasmid was determined using PacBio RSII and Roche 454 sequencing. (C) 2015 Elsevier B.V. All rights reserved.
Accession Number: WOS:000365364900022
PubMed ID: 26410453
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sedlar, Karel	K-1120-2014	0000-0002-8269-4020
Patakova, Petra	B-6404-2018	0000-0002-9410-4454
Skutkova, Helena	D-5194-2014	0000-0003-4562-2746
Provaznik, Ivo	F-4121-2012	0000-0002-3422-7938

ISSN: 0168-1656
eISSN: 1873-4863

Record 395 of 491
Title: Dipole response in Pb-208 within a self-consistent multiphonon approach
Author(s): Knapp, F (Knapp, F.); Lo Iudice, N (Lo Iudice, N.); Vesely, P (Vesely, P.); Andreozzi, F (Andreozzi, F.); De Gregorio, G (De Gregorio, G.); Porrino, A (Porrino, A.)
Source: PHYSICAL REVIEW C **Volume:** 92 **Issue:** 5 **Article Number:** 054315 **DOI:** 10.1103/PhysRevC.92.054315 **Published:** NOV 18 2015
Abstract: Background: The electric dipole strength detected around the particle threshold and commonly associated with the pygmy dipole resonance offers unique information on neutron skin and symmetry energy, and is of astrophysical interest. The nature of such a resonance is still under debate.
Purpose: We intend to describe the giant and pygmy resonances in Pb-208 by enhancing their fragmentation with respect to the random-phase approximation.
Method: We adopt the equation of motion phonon method to perform a fully self-consistent calculation in a space spanned by one-phonon and two-phonon basis states using an optimized chiral two-body potential. A phenomenological density-dependent term, derived from a contact three-body force, is added to get single-particle spectra more realistic than the ones obtained by using the chiral potential only. The calculation takes into full account the Pauli principle and is free of spurious center-of-mass admixtures.
Results: We obtain a fair description of the giant resonance and obtain a dense low-lying spectrum in qualitative agreement with the experimental data. The transition densities as well as the phonon and particle-hole composition of the most strongly excited states support the pygmy nature of the low-lying resonance. Finally, we obtain realistic values for the dipole polarizability and the neutron skin radius.
Conclusions: The results emphasize the role of the two-phonon states in enhancing the fragmentation of the strength in the giant resonance region and at low energy, consistently with experiments. For a more detailed agreement with the data, the calculation suggests the inclusion of the three-phonon states as well as a fine tuning of the single-particle spectrum to be obtained by a refinement of the nuclear potential.
Accession Number: WOS:000364901400001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290
De Gregorio, Giovanni		0000-0003-0253-915X
Lo Iudice, Nicola		0000-0003-2662-2054

ISSN: 0556-2813
eISSN: 1089-490X

Record 396 of 491

Title: Computational study of productive and non-productive cycles in fluoroalkene metathesis
Author(s): Rybackova, M (Rybackova, Marketa); Hosek, J (Hosek, Jan); Simunek, O (Simunek, Ondrej); Kolarikova, V (Kolarikova, Viola); Kvicala, J (Kvicala, Jaroslav)
Source: BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY **Volume:** 11 **Pages:** 2150-2157 **DOI:** 10.3762/bjoc.11.232 **Published:** NOV 10 2015
Abstract: A detailed DFT study of the mechanism of metathesis of fluoroethene, 1-fluoroethene, 1,1-difluoroethene, cis- and trans-1,2-difluoroethene, tetrafluoroethene and chlorotrifluoroethene catalysed with the Hoveyda-Grubbs 2nd generation catalyst was performed. It revealed that a successful metathesis of hydrofluoroethenes is hampered by a high preference for a non-productive catalytic cycle proceeding through a ruthenacyclobutane intermediate bearing fluorines in positions 2 and 4. Moreover, the calculations showed that the cross-metathesis of perfluoro-or perhaloalkenes should be a feasible process and that the metathesis is not very sensitive to stereochemical issues.
Accession Number: WOS:000364364300002
PubMed ID: 26664636
ISSN: 1860-5397

Record 397 of 491
Title: Comparing XMCD and DFT with STM spin excitation spectroscopy for Fe and Co adatoms on Cu2N/Cu(100)
Author(s): Etzkorn, M (Etzkorn, M.); Hirjibehedin, CF (Hirjibehedin, C. F.); Lehnert, A (Lehnert, A.); Ouazi, S (Ouazi, S.); Rusponi, S (Rusponi, S.); Stepanow, S (Stepanow, S.); Gambardella, P (Gambardella, P.); Tieg, C (Tieg, C.); Thakur, P (Thakur, P.); Lichtenstein, AI (Lichtenstein, A. I.); Shick, AB (Shick, A. B.); Loth, S (Loth, S.); Heinrich, AJ (Heinrich, A. J.); Brune, H (Brune, H.)
Source: PHYSICAL REVIEW B **Volume:** 92 **Issue:** 18 **Article Number:** 184406 **DOI:** 10.1103/PhysRevB.92.184406 **Published:** NOV 5 2015
Abstract: We report on the magnetic properties of Fe and Co adatoms on a Cu2N/Cu(100)-c(2 x 2) surface investigated by x-ray magnetic dichroism measurements and density functional theory (DFT) calculations including the local coulomb interaction. We compare these results with properties formerly deduced from STM spin excitation spectroscopy (SES) performed on the individual adatoms. In particular we focus on the values of the local magnetic moments determined by XMCD compared to the expectation values derived from the description of the SES data. The angular dependence of the projected magnetic moments along the magnetic field, as measured by XMCD, can be understood on the basis of the SES Hamiltonian. In agreement with DFT, the XMCD measurements show large orbital contributions to the total magnetic moment for both magnetic adatoms.
Accession Number: WOS:000364158900005
Author Identifiers:

Author	ResearcherID Number	ORCID Number
EPFL, Physics	O-6514-2016	
Lichtenstein, Alexander	K-8730-2012	0000-0003-0152-7122
Brune, Harald	E-7284-2017	0000-0003-4459-3111
Shick, Alexander	C-1420-2013	0000-0003-2700-5517
Thakur, Pardeep Kumar	A-8328-2012	0000-0002-9599-0531
Hirjibehedin, Cyrus		0000-0003-1706-2147
Rusponi, Stefano		0000-0002-8494-5532

ISSN: 1098-0121
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Record 398 of 491
Title: Multiple displacement amplification of the DNA from single flow-sorted plant chromosome
Author(s): Capal, P (Capal, Petr); Blavet, N (Blavet, Nicolas); Vrana, J (Vrana, Jan); Kubalakova, M (Kubalakova, Marie); Dolezel, J (Dolezel, Jaroslav)
Source: PLANT JOURNAL **Volume:** 84 **Issue:** 4 **Pages:** 838-844 **DOI:** 10.1111/tpj.13035 **Published:** NOV 2015
Abstract: A protocol is described for production of micrograms of DNA from single copies of flow-sorted plant chromosomes. Of 183 single copies of wheat chromosome 3B, 118 (64%) were successfully amplified. Sequencing DNA amplification products using an Illumina HiSeq 2000 system to 103 coverage and merging sequences from three separate amplifications resulted in 60% coverage of the chromosome 3B reference, entirely covering 30% of its genes. The merged sequences permitted de novo assembly of 19% of chromosome 3B genes, with 10% of genes contained in a single contig, and 39% of genes covered for at least 80% of their length. The chromosome-derived sequences allowed identification of missing genic sequences in the chromosome 3B reference and short sequences similar to 3B in survey sequences of other wheat chromosomes. These observations indicate that single-chromosome sequencing is suitable to identify genic sequences on particular chromosomes, to develop chromosome-specific DNA markers, to verify assignment of DNA sequence contigs to individual pseudomolecules, and to validate whole-genome assemblies. The protocol expands the potential of chromosome genomics, which may now be applied to any plant species from which chromosome samples suitable for flow cytometry can be prepared, and opens new avenues for studies on chromosome structural heterozygosity and haplotype phasing in plants.
Accession Number: WOS:000368259100016
PubMed ID: 26400218
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vrana, Jan	F-7306-2014	0000-0001-6171-8516
Blavet, Nicolas	F-8148-2014	0000-0003-2199-9119

ISSN: 0960-7412
eISSN: 1365-313X

Record 399 of 491
Title: Evolution of laser induced electromagnetic postsolitons in multi-species plasma
Author(s): Liu, Y (Liu, Yue); Klimo, O (Klimo, Ondrej); Esirkepov, TZ (Esirkepov, Timur Zh.); Bulanov, SV (Bulanov, Sergei V.); Gu, YJ (Gu, Yanjun); Weber, S (Weber, Stefan); Korn, G (Korn, Georg)
Source: PHYSICS OF PLASMAS **Volume:** 22 **Issue:** 11 **Article Number:** 112302 **DOI:** 10.1063/1.4935303 **Published:** NOV 2015
Abstract: The evolution of an s-polarized relativistic electromagnetic soliton created in multi-species plasma by an intense short laser pulse is investigated using two-dimensional particle-in-cell simulations. The multi-component plasma consists of electrons and high-Z ions with a small addition of protons. By comparison, the evolution of postsoliton is very different from that in hydrogen plasma. A halo-like structure is found in spatial patterns of both electromagnetic fields and electron densities. The process of energy depletion is much slower due to the smaller charge-to-mass ratio of ions, which implies a better way of detecting postsolitons in simulations and experiments. In addition, it is found that the Coulomb explosion of high-Z ions in the postsoliton stage facilitates low-Z ion acceleration, and the maximum energy of low-Z ions increases with the component ratio of high-Z to low-Z ions. (C) 2015 AIP Publishing LLC.
Accession Number: WOS:000366054900026
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Klimo, Ondrej	B-2196-2010	0000-0002-0565-2409
Esirkepov, Timur		0000-0002-9027-0703

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Record 400 of 491
Title: THE ORIGIN OF PROLATE ROTATION IN DWARF SPHEROIDAL GALAXIES FORMED BY MERGERS OF DISKY DWARFS
Author(s): Ebrova, I (Ebrova, Ivana); Lokas, EL (Lokas, Ewa L.)
Source: ASTROPHYSICAL JOURNAL **Volume:** 813 **Issue:** 1 **Article Number:** 10 **DOI:** 10.1088/0004-637X/813/1/10 **Published:** NOV 1 2015
Abstract: Motivated by the discovery of prolate rotation of stars in Andromeda II (And II), a dwarf spheroidal companion of M31, we study its origin via mergers of disky dwarf galaxies. We simulate merger events between two identical dwarfs changing the initial inclination of their disks with respect to the orbit and the amount of orbital angular momentum. On radial orbits, the amount of prolate rotation in the merger remnants correlates strongly with the inclination of the disks and is well understood as due to the conservation of the angular momentum component of the disks along the merger axis. For non-radial orbits, prolate rotation may still be produced if the orbital angular momentum is initially not much

larger than the intrinsic angular momentum of the disks. The orbital structure of the remnants with significant rotation is dominated by box orbits in the center and long-axis tubes in the outer parts. The frequency analysis of stellar orbits in the plane perpendicular to the major axis reveals the presence of two families roughly corresponding to inner and outer long-axis tubes. The fraction of inner tubes is largest in the remnant forming from disks that are initially oriented most vertically, and is responsible for the boxy shape of the galaxy. We conclude that prolate rotation results from mergers with a variety of initial conditions and no fine tuning is necessary to reproduce this feature. We compare the properties of our merger remnants to those of dwarfs resulting from the tidal stirring scenario and the data for And II.

Accession Number: WOS:000365284100010

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Lokas, Ewa		0000-0001-7138-8899

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Page 9 (Records 401 -- 450)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 401 of 491

Title: Scrimer: designing primers from transcriptome data

Author(s): Morkovsky, L (Morkovsky, Libor); Paces, J (Paces, Jan); Ridl, J (Ridl, Jakub); Reifova, R (Reifova, Radka)

Source: MOLECULAR ECOLOGY RESOURCES **Volume:** 15 **Issue:** 6 **Pages:** 1415-1420 **DOI:** 10.1111/1755-0998.12403 **Published:** NOV 2015

Abstract: With the rise of next-generation sequencing methods, it has become increasingly possible to obtain genomewide sequence data even for nonmodel species. Such data are often used for the development of single nucleotide polymorphism (SNP) markers, which can subsequently be screened in a larger population sample using a variety of genotyping techniques. Many of these techniques require appropriate locus-specific PCR and genotyping primers. Currently, there is no publicly available software for the automated design of suitable PCR and genotyping primers from next-generation sequence data. Here we present a pipeline called Scrimer that automates multiple steps, including adaptor removal, read mapping, selection of SNPs and multiple primer design from transcriptome data. The designed primers can be used in conjunction with several widely used genotyping methods such as SNaPshot or MALDI-TOF genotyping. Scrimer is composed of several reusable modules and an interactive bash workflow that connects these modules. Even the basic steps are presented, so the workflow can be executed in a step-by-step manner. The use of standard formats throughout the pipeline allows data from various sources to be plugged in, as well as easy inspection of intermediate results with visualization tools of the user's choice.

Accession Number: WOS:000362838300015

PubMed ID: 25773304

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reifova, Radka	D-2137-2011	0000-0001-5852-5174
Paces, Jan	C-8851-2009	0000-0003-3059-6127

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eISSN: 1755-0998

Record 402 of 491

Title: Solid-state deep blue and UV fluorescent dyes based on para-bis(2-thienyl)phenylene

Author(s): Krajcovic, J (Krajcovic, Jozef); Kovalenko, A (Kovalenko, Alexander); Heinrichova, P (Heinrichova, Patricie); Vala, M (Vala, Martin); Weiter, M (Weiter, Martin)

Source: JOURNAL OF LUMINESCENCE **Volume:** 167 **Pages:** 222-226 **DOI:** 10.1016/j.jlumin.2015.06.043 **Published:** NOV 2015

Abstract: Despite the general rule of strong acceptor substituents having a tendency to quench fluorescence due to molecular stacking, it is shown how tetra-fluorination of the central phenylene unit of para-bis(2-thienyl)phenylene can augment the quantum yields of solid state fluorescent dyes. Another significant part of the present research was the study of the influence of the position of the solubilization alkyl chains position on the fluorescent properties of the above mentioned non- and tetra-fluorinated materials. Tenfold augmentation of quantum yields, depending on the position of the alkyl chains is reported. (C) 2015 Elsevier B.V. All rights reserved.

Accession Number: WOS:000361401600033

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vala, Martin	A-1489-2009	0000-0003-2229-6669
Weiter, Martin	A-8250-2016	
Krajcovic, Jozef	D-5240-2013	
Kovalenko, Alexander	A-7336-2016	

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Record 403 of 491

Title: Modified Becke-Johnson (mBJ) exchange potential investigations of the optoelectronic structure of the quaternary diamond-like semiconductors Li2CdGeS4 and Li2CdSnS4

Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Goumri-Said, S (Goumri-Said, Souraya)

Source: MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING **Volume:** 39 **Pages:** 606-613 **DOI:** 10.1016/j.mssp.2015.05.068 **Published:** NOV 2015

Abstract: Li2CdGeS4 and Li2CdSnS4 compounds are diamond-like semiconductors (DLSs) and have been investigated to explore their electronic structure and optical properties for potential optoelectronic applications. Density functional theory within the modified Becke-Johnson (mBJ) exchange potential shows that the band structures exhibit direct band gap semiconductors at Gamma with optical band gaps of 2.461 and 3.16 eV for Li2CdGeS4 and Li2CdSnS4 respectively. Along side showing that both compounds are optically active materials, our finding exhibit a nice harmony with experimental measured band gaps (3.10 eV and 3.26 eV for Li2CdGeS4 and Li2CdSnS4). Charge densities iso-surfaces and two-dimensional maps were reported to determine the effect of Sn/Ge on the bonding characteristics of both DLSs. The static dielectric constant epsilon(1)(0) and static refractive index n(0) are decreasing when Ge is replaced by Sn. Consequently, the possibility to tune the band gap for both DISs could lead us to target particular optoelectronic applications in the next future such LED and solar cells. (C) 2015 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000361774100083

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Azam, Sikander		0000-0001-5923-1127

ISSN: 1369-8001

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Record 404 of 491

Title: Ab initio study of atomic disorder on As-rich GaAs(111)A surface

Author(s): Romanyuk, O (Romanyuk, O.); Mutombo, P (Mutombo, P.); Grosse, F (Grosse, F.)

Source: SURFACE SCIENCE **Volume:** 641 **Pages:** 330-335 **DOI:** 10.1016/j.susc.2015.01.015 **Published:** NOV 2015

Abstract: Mechanisms for the appearance of disorder on the As-rich GaAs (111)A surface were investigated employing density functional theory (DFT). Focus was given to the As trimer interactions by considering different surface symmetries and rest site occupations. The (2 x 2) and the c(4 x 2) structure models with As trimer and an As rest site were found the most energetically stable under the As-rich experimental conditions at T = 0 K. Low interactions between neighboring As trimers causes disorder in thermodynamic equilibrium at finite temperatures. A careful analysis of the configurational entropy contributions including the different statistics was carried out. The experimentally observed As-rich (2 x 2) structure was confirmed to be kinetically stabilized. The stabilization mechanism is discussed with respect to the As trimer migration on the surface, which is limited by a large diffusion barrier through the As rest sites. (C) 2015 Elsevier B.V. All rights reserved.

Accession Number: WOS:000361408800054

Conference Title: European Conference on Surface Science (ECOSS)

Conference Date: AUG 31-SEP 05, 2014

Conference Location: Antalya, TURKEY

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Mutombo, Pingo		0000-0002-8175-7587
Romanyuk, Oleksandr		0000-0003-0430-3706

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Record 405 of 491

Title: Fast magnetic field annihilation driven by two laser pulses in underdense plasma

Author(s): Gu, YJ (Gu, Y. J.); Klimo, O (Klimo, O.); Kumar, D (Kumar, D.); Bulanov, SV (Bulanov, S. V.); Esirkepov, TZ (Esirkepov, T. Zh.); Weber, S (Weber, S.); Korn, G (Korn, G.)

Source: PHYSICS OF PLASMAS **Volume:** 22 **Issue:** 10 **Article Number:** 103113 **DOI:** 10.1063/1.4933408 **Published:** OCT 2015

Abstract: Fast magnetic annihilation is investigated by using 2.5-dimensional particle-in-cell simulations of two parallel ultra-short petawatt laser pulses co-propagating in underdense plasma. The magnetic field generated by the laser pulses annihilates in a current sheet formed between the pulses. Magnetic field energy is converted to an inductive longitudinal electric field, which efficiently accelerates the electrons of the current sheet. This new regime of collisionless relativistic magnetic field annihilation with a timescale of tens of femtoseconds can be extended to near-critical and overdense plasma with the ultra-high intensity femtosecond laser pulses. (C) 2015 AIP Publishing LLC.

Accession Number: WOS:000364403600083

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Gu, Yanjun	G-5767-2014	0000-0002-6234-8489
Bulanov, Sergei	A-1721-2013	
Klimo, Ondrej	B-2196-2010	0000-0002-0565-2409
Kumar, Deepak	J-3614-2015	
Esirkepov, Timur		0000-0002-9027-0703

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Record 406 of 491

Title: Molecular phylogeny of the Bothriocephalidea (Cestoda): molecular data challenge morphological classification

Author(s): Brabec, J (Brabec, Jan); Waeschenbach, A (Waeschenbach, Andrea); Scholz, T (Scholz, Tomg); Littlewood, DTJ (Littlewood, D. Timothy J.); Kuchta, R (Kuchta, Roman)

Source: INTERNATIONAL JOURNAL FOR PARASITOLOGY **Volume:** 45 **Issue:** 12 **Pages:** 761-771 **DOI:** 10.1016/j.ijpara.2015.05.006 **Published:** OCT 2015

Abstract: In this study, the relationships of the cestode order Bothriocephalidea, parasites of marine and freshwater bony fish, were assessed using multi-gene molecular phylogenetic analyses. The dataset included 59 species, covering approximately 70% of currently recognised genera, a sample of bothriocephalidean biodiversity gathered through an intense 15 year effort. The order as currently circumscribed, while monophyletic, includes three non-monophyletic and one monophyletic families. Bothriocephalidae is monophyletic and forms the most derived lineage of the order, comprised of a single freshwater and several marine clades. Biogeographic patterns within the freshwater clade are indicative of past radiations having occurred in Africa and North America. The earliest diverging lineages of the order comprise a paraphyletic Triaenophoridae. The Echinophallidae, consisting nearly exclusively of parasites of pelagic fish, was also resolved as paraphyletic with respect to the Bothriocephalidae. Philobythoides sp., the only representative included from the Philobythiidae, a unique family of parasites of bathypelagic fish, was sister to the genus Eubothrium, the latter constituting one of the lineages of the paraphyletic Triaenophoridae. Due to the weak statistical support for most of the basal nodes of the Triaenophoridae and Echinophallidae, as well as the lack of obvious morphological synapomorphies shared by taxa belonging to the statistically well-supported lineages, the current family-level classification, although mostly non-monophyletic, is provisionally retained, with the exception of the family Philobythiidae, which is recognised as a synonym of the Triaenophoridae. In addition, Schyzocotyle is resurrected to accommodate the invasive Asian fish tapeworm, Schyzocotyle acheilognathi (Yamaguti, 1934) n. comb. (syn. Bothriocephalus acheilognathi Yamaguti, 1934), which is of veterinary importance, and Schyzocotyle nayarensis (Malhotra, 1983) n. comb. (syn. Ptychobothrium nayarensis Malhotra, 1983). The genus is morphologically characterised by a wide, heart-shaped scolex with narrow, deep bothria. (C) 2015 Australian Society for Parasitology Inc. Published by Elsevier Ltd. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kuchta, Roman	H-7828-2012	0000-0002-4219-6924
Scholz, Tomas	G-8360-2014	0000-0002-6340-3750
Littlewood, Tim	B-5230-2008	0000-0002-2718-4001
Brabec, Jan	G-8419-2014	0000-0002-2636-414X

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Record 407 of 491

Title: DFT and modified Becke Johnson (mBJ) potential investigations of the optoelectronic properties of SnGa(4)Q(7) (Q = S, Se) compounds: Transparent materials for large energy conversion

Author(s): Khan, W (Khan, Wilayat); Azam, S (Azam, Sikander); Shah, FA (Shah, Fahad Ali); Goumri-Said, S (Goumri-Said, Souraya)

Source: SOLID STATE SCIENCES **Volume:** 48 **Pages:** 244-250 **DOI:** 10.1016/j.solidstatesciences.2015.08.015 **Published:** OCT 2015

Abstract: Electronic structure and optical properties of SnGa(4)Q(7) (Q = S, Se) compounds were investigated using a full potential linearized augmented plane wave method based on density functional formalism. Electronic band structures show an indirect semiconducting wide band gap two different approaches (EVGGA and mBJ). The band gap values are estimated at 2.90 (2.25 eV) and 3.11 (2.49 eV) for EV-CGA and mBJ for SnGa(4)Q(7) (SnGa(4)Q(7)), respectively. Densities of states show that Sn-5s and S/Se-3p/4p states are dominating the region around Fermi level form valence band maximum and conduction band minimum. The computed electronic charge density contours demonstrate that SnGa(4)Q(7) (Q = S, Se) show a mixture between ionic and covalent characters. Optical parameters including the dielectric constant, absorption coefficient, reflectivity, refractive index, energy loss function, and birefringence are also reported to investigate the potential role of SnGa(4)Q(7) (Q = S, Se) compounds for solar energy conversion application. (C) 2015 Elsevier Masson SAS. All rights reserved.

Accession Number: WOS:000363347800037

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Azam, Sikander		0000-0001-5923-1127

ISSN: 1293-2558

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Record 408 of 491

Title: Different Response of Carbonyl Carotenoids to Solvent Proticity Helps To Estimate Structure of the Unknown Carotenoid from Chromera velia

Author(s): Kesan, G (Kesan, Guerkan); Durchan, M (Durchan, Milan); Tichy, J (Tichy, Josef); Minofar, B (Minofar, Babak); Kuznetsoya, V (Kuznetsoya, Valentyna); Fuciman, M (Fuciman, Marcel); Slouf, V (Slouf, Vaclav); Parlak, C (Parlak, Cemal); Polivka, T (Polivka, Tomas)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 119 **Issue:** 39 **Pages:** 12653-12663 **DOI:** 10.1021/acs.jpcb.5b08152 **Published:** OCT 1 2015

Abstract: In order to estimate the possible structure of the unknown carbonyl carotenoid related to isofucoxanthin from Chromera velia denoted as isofucoxanthin-like carotenoid (Ifx-l), we employed steady-state and ultrafast time-resolved spectroscopic techniques to investigate spectroscopic properties of Ifx-l in various solvents. The results were compared with those measured for related carotenoids with luiown structure: fucoxanthin (Fx) and isofucoxanthin (la). The experimental data were complemented by quantum chemistry calculations and molecular modeling. The data show that Ifx-l must have longer effective conjugation length than Ifx. Yet, the magnitude of polarity-dependent changes in Ifx-l is larger than for Ifx suggesting significant differences in structure of these two carotenoids. The most interesting spectroscopic feature of Ifx-1 is its response to solvent proticity. The transient absorption data show that (1) the magnitude of the ICT-like band of Ifx-l in acetonitrile is larger than in methanol and (2) the S-1/ICT lifetime of Ifx-l in acetonitrile, 4 ps, is markedly shorter than in methanol (10 ps). This is opposite behavior than for Fx and Ifx whose S-1/ICT lifetimes are always shorter in protic solvent methanol (20 and 13 ps) than in aprotic acetonitrile (30 and 17 ps). Comparison with other carbonyl carotenoids reported earlier showed that proticity response of Ifx-l is consistent with presence of a conjugated lactone ring. Combining the experimental data and quantum chemistry calculations, we estimated a possible structure of Ifx-l.

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PubMed ID: 26362118
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Durchan, Milan	G-9464-2014	
Polivka, Tomas	G-9564-2014	0000-0002-6176-0420
KESAN, Gurkan	G-4760-2012	0000-0002-4173-8250
Minofar, Babak	D-7361-2016	

ISSN: 1520-6106

Record 409 of 491
Title: Coulomb interaction and spin-orbit coupling calculations of thermoelectric properties of the quaternary chalcogenides Tl2PbXY4 (X = Zr, Hf and Y = S, Se)
Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Minar, J (Minar, Jan); Khan, W (Khan, Wilayat); Din, HU (Din, Haleem Ud); Khenata, R (Khenata, R.); Murtaza, G (Murtaza, G.); Bin-Omran, S (Bin-Omran, S.); Goumri-Said, S (Goumri-Said, Souraya)
Source: SEMICONDUCTOR SCIENCE AND TECHNOLOGY **Volume:** 30 **Issue:** 10 **Article Number:** 105018 **DOI:** 10.1088/0268-1242/30/10/105018 **Published:** OCT 2015
Abstract: The increase in energy demands is leading to growing interest in new thermoelectric inorganic materials, such as the chalcogenides. The recently synthesized quaternary chalcogenide, Tl2PbXY4 (X = Zr, Hf and Y = S, Se), compounds were investigated using the full potential linear augmented plane wave method based on density functional theory. We used the generalized gradient approximation plus the optimized effective Hubbard parameter U to treat the exchange correlation. The existence of heavy metals (Tl, Pb and Hf) required the application of relativistic spin-orbit coupling via a second variational procedure. Tl2PbHfS4, Tl2PbHfSe4, Tl2PbZrS4 and Tl2PbZrSe4 compounds were found to be semiconductors with indirect band gaps of 0.911, 0.659, 0.983 and 0.529 eV, respectively. The types of carriers and electrical transport properties of Tl2PbXY4 (X = Zr, Hf and Y = S, Se) are attributed to the Tl-d and S/Se-s electronic states near the Fermi level. Optical properties were investigated via the calculation of dielectric function and reflectivity. Using Boltzmann theory, we compared the thermoelectric properties and we found that Tl2PbHfS4 could be a good candidate for thermoelectric devices.
Accession Number: WOS:000362602300026
Author Identifiers:

Author	ResearcherID Number	ORCID Number
BINOMRAN, SAAD	N-7968-2016	0000-0001-6097-2344
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Minar, Jan	O-3186-2013	0000-0001-9735-8479
Azam, Sikander		0000-0001-5923-1127

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Record 410 of 491
Title: Calculation of cellular S-values using Geant4-DNA: The effect of cell geometry
Author(s): Sefl, M (Sefl, Martin); Incerti, S (Incerti, Sebastien); Papamichael, G (Papamichael, George); Emfietzoglou, D (Emfietzoglou, Dimitris)
Source: APPLIED RADIATION AND ISOTOPES **Volume:** 104 **Pages:** 113-123 **DOI:** 10.1016/j.apradiso.2015.06.027 **Published:** OCT 2015
Abstract: Purpose: Geant4-DNA is used to calculate S-values for different subcellular distributions of low-energy electron sources in various cell geometries.
Method: Calculations of cellular S-values for monoenergetic electron sources with energy from 1 to 100 keV and the Auger-electron emitting radionuclides Tc-99m, In-111, and I-125 have been made using the Geant4 Monte Carlo toolkit. The Geant4-DNA low-energy extension is employed for simulating collision-by-collision the complete slowing-down of electron tracks (down to 8 eV) in liquid water, used as a surrogate of human cells. The effect of cell geometry on S-values is examined by simulating electron tracks within different cell geometries, namely, a spherical, two ellipsoidal, and an irregular shape, all having equal cellular and nuclear volumes. Algorithms for randomly sampling the volume of the nucleus, cytoplasm, surface, and whole cell for each cell phantom are presented.
Results: Differences between Geant4-DNA and MIRD database up to 50% were found, although, for the present radionuclides, they mostly remain below 10%. For most source-target combinations the S-values for the spherical cell geometry were found to be within 20% of those for the ellipsoidal cell geometries, with a maximum deviation of 32%. Differences between the spherical and irregular geometries are generally larger reaching 100-300%. Most sensitive to the cell geometry is the absorbed dose to the nucleus when the source is localized on the cell surface. Interestingly, two published AAPM spectra for 1-125 yield noticeable differences (up to 19%) in cellular S-values.
Conclusion: Monte Carlo simulations of cellular S-values with Geant4-DNA reveal that, for the examined radionuclides, the widely used approximation of spherical cells is reasonably accurate (within 20-30%) even for ellipsoidal geometries. For irregular cell geometries the spherical approximation should be used with caution because, as in the present example, it may lead to erroneous results for the nuclear dose for the commonly encountered situation where the source is localized to the cell surface. (C) 2015 Elsevier Ltd. All rights reserved.
Accession Number: WOS:000360948600016
PubMed ID: 26159660
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Emfietzoglou, Dimitris	G-7168-2012	
Incerti, Sebastien	T-3006-2017	0000-0002-0619-2053
Sefl, Martin		0000-0003-2164-6620

ISSN: 0969-8043

Record 411 of 491
Title: Exploring the electronic structure and optical properties of new inorganic luminescent materials Ba(Si,Al)(5)(O,N)(8) compounds for light-emitting diodes devices
Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Minar, J (Minar, Jan); Goumri-Said, S (Goumri-Said, Souraya)
Source: CURRENT APPLIED PHYSICS **Volume:** 15 **Issue:** 10 **Pages:** 1160-1167 **DOI:** 10.1016/j.cap.2015.06.025 **Published:** OCT 2015
Abstract: Due to growing demand on discovering new materials for light-emitting diodes devices, many efforts were made to discover and characterize new inorganic materials such as phosphors. Using the full potential method within density functional theory the electronic and optical properties of BaAl2Si3O4N4 and BaAlSi4O3N5 semiconductors have been investigated. The electronic structure and the optical properties of these phosphors were calculated through a reliable approach of modified Beck-Johnson (mBJ) approach. We found that BaAl2Si3O4N4 and BaAlSi4O3N5 have wide direct band gaps positioned at G about 5.846 and 4.96 eV respectively. The optical properties, namely the dielectric function, optical reflectivity, refractive index and electron energy loss, are reported for radiation up to 15 eV. Our study suggests that BaAl2Si3O4N4 and BaAlSi4O3N5 could be promising materials for applications in the LEDs devices and optoelectronics areas of research. (C) 2015 Elsevier B.V. All rights reserved.
Accession Number: WOS:000360915500011
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Minar, Jan	O-3186-2013	0000-0001-9735-8479
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Azam, Sikander		0000-0001-5923-1127

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Record 412 of 491
Title: Exploring W-infinity in the quadratic basis
Author(s): Prochazka, T (Prochazka, Tomas)
Source: JOURNAL OF HIGH ENERGY PHYSICS **Issue:** 9 **Article Number:** 116 **DOI:** 10.1007/JHEP09(2015)116 **Published:** SEP 17 2015

Abstract: We study the operator product expansions in the chiral algebra W-infinity, first using the associativity conditions in the basis of primary generating fields and then using a different basis coming from the free field representation in which the OPE takes a simpler quadratic form. The results in the quadratic basis can be compactly written using certain bilocal combinations of the generating fields and we conjecture a closed-form expression for the complete OPE in this basis. Next we show that the commutation relations as well as correlation functions can be easily computed using properties of these bilocal fields. In the last part we verify the consistency with results derived previously by studying minimal models of W-infinity and comparing them to known reductions of W-infinity to W-N. The results we obtain illustrate nicely the role of triality symmetry in the representation theory of W-infinity

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Record 413 of 491

Title: PoisFFT - A free parallel fast Poisson solver

Author(s): Fuka, V (Fuka, V.)

Source: APPLIED MATHEMATICS AND COMPUTATION **Volume:** 267 **Pages:** 356-364 **DOI:** 10.1016/j.amc.2015.03.011 **Published:** SEP 15 2015

Abstract: A fast Poisson solver software package PoisFFT is presented. It is available as a free software licensed under the GNU GPL license version 3. The package uses the fast Fourier transform to directly solve the Poisson equation on a uniform orthogonal grid. It can solve the pseudo-spectral approximation and the second order finite difference approximation of the continuous solution. The paper reviews the mathematical methods for the fast Poisson solver and discusses the software implementation and parallelization. The use of PoisFFT in an incompressible flow solver is also demonstrated. (C) 2015 Published by Elsevier Inc.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fuka, Vladimir	P-1447-2017	0000-0001-8712-2892

ISSN: 0096-3003

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Record 414 of 491

Title: Singles correlation energy contributions in solids

Author(s): Klimes, J (Klimes, Jiri); Kaltak, M (Kaltak, Merzuk); Maggio, E (Maggio, Emanuele); Kresse, G (Kresse, Georg)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 143 **Issue:** 10 **Article Number:** 102816 **DOI:** 10.1063/1.4929346 **Published:** SEP 14 2015

Abstract: The random phase approximation to the correlation energy often yields highly accurate results for condensed matter systems. However, ways how to improve its accuracy are being sought and here we explore the relevance of singles contributions for prototypical solid state systems. We set out with a derivation of the random phase approximation using the adiabatic connection and fluctuation dissipation theorem, but contrary to the most commonly used derivation, the density is allowed to vary along the coupling constant integral. This yields results closely paralleling standard perturbation theory. We re-derive the standard singles of Gorling-Levy perturbation theory [A. Gorling and M. Levy, Phys. Rev. A 50, 196 (1994)], highlight the analogy of our expression to the renormalized singles introduced by Ren and coworkers [Phys. Rev. Lett. 106, 153003 (2011)], and introduce a new approximation for the singles using the density matrix in the random phase approximation. We discuss the physical relevance and importance of singles alongside illustrative examples of simple weakly bonded systems, including rare gas solids (Ne, Ar, Xe), ice, adsorption of water on NaCl, and solid benzene. The effect of singles on covalently and metallically bonded systems is also discussed. (C) 2015 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution 3.0 Unported License.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Klimes, Jiri	D-8926-2011	0000-0003-4969-1343

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Record 415 of 491

Title: Charge localization and magnetocrystalline anisotropy in La, Pr, and Nd substituted Sr hexaferrites

Author(s): Chlan, V (Chlan, Vojtech); Kouril, K (Kouril, Karel); Ulicna, K (Ulicna, Katerina); Stepankova, H (Stepankova, Helena); Topfer, J (Toepfer, Jorg); Seifert, D (Seifert, Daniela)

Source: PHYSICAL REVIEW B **Volume:** 92 **Issue:** 12 **Article Number:** 125125 **DOI:** 10.1103/PhysRevB.92.125125 **Published:** SEP 14 2015

Abstract: Charge compensation in strontium M-type hexaferrites A(x)(3+)Sr(1-x)Fe(12)O(19) (A = La, Nd, or Pr) is studied by means of calculations of electronic structure and Fe-57 nuclear magnetic resonance (NMR) experiments. Two different states are realized in the calculations: a localized scenario as a ground state with the extra valence charge preferentially in the octahedral 2a sites and a delocalized scenario with the charge delocalized over multiple sites. From the calculations and NMR experiments, it is deduced that the localized state Fe2+(2a) occurs at low temperatures regardless of the type of used substitution and that the distribution of ferric and ferrous ions within the 2a sublattice is static at low temperatures. The magnetocrystalline anisotropy energy of Sr and La hexaferrites is calculated and the contributions of individual Fe sublattices are evaluated. The temperature dependence of the anisotropy for La hexaferrite is explained as a transition between localized and delocalized states causing changes in the single ion contributions of Fe in 2a and also 12k sites.

Accession Number: WOS:000361118600007

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Chlan, Vojtech	D-4868-2017	0000-0001-6963-9273
Stepankova, Helena	P-2352-2017	0000-0002-4051-2495
Kouril, Karel		0000-0003-4884-1637

ISSN: 2469-9950

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Record 416 of 491

Title: Rapid theory-guided prototyping of ductile Mg alloys: from binary to multi-component materials

Author(s): Pei, ZR (Pei, Zongrui); Friak, M (Friak, Martin); Sandlobes, S (Sandloebes, Stefanie); Nazarov, R (Nazarov, Roman); Svendsen, B (Svendsen, Bob); Raabe, D (Raabe, Dierk); Neugebauer, J (Neugebauer, Joerg)

Source: NEW JOURNAL OF PHYSICS **Volume:** 17 **Article Number:** 093009 **DOI:** 10.1088/1367-2630/17/9/093009 **Published:** SEP 9 2015

Abstract: In order to identify a method allowing for a fast solute assessment without lengthy ab initio calculations, we analyze correlations and anti-correlation between the I-1 stacking fault energies (I-1 SFEs), which were shown to be related to the macroscopic ductility in Mg alloys, and five material parameters of 18 different elemental solutes. Our analysis reveals that the atomic volume V of pure solutes, their electronegativity. and bulk modulus B are either linearly or logarithmically related to the I-1 SFE. Comparing the impact of solutes with that of yttrium (that increases the ductility in Mg) we propose a single numerical quantity (called yttrium similarity index, YSI) that is based on these interrelations. Subsequently, we evaluate this new figure of merit for 76 elements from the periodic table of elements in search for solutes reducing the I-1 SFE. Limiting ourselves first to binary Mg alloys, we hardly find any alternative solutes providing similar I1SFE reduction as that due to rare-earth (RE) additions. Therefore, we extended our search to ternary Mg alloys. Assuming that the physical properties of solute combinations can be represented by their average values, 2850 solute combinations were checked and 133 solute pairs (not including any RE elements) have been found to have a YSI larger than 0.85. Quantum-mechanical calculations have been subsequently performed for 11 solute pairs with YSIs higher than 0.95 and they were all found to reduce the I1SFE in excellent agreement with the predictions based on the YSI.

Accession Number: WOS:000367355600005
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Neugebauer, Joerg	K-2041-2015	0000-0002-7903-2472
Svendsen, Bob	D-6311-2014	0000-0002-1519-9433
Pei, Zongrui		0000-0003-0748-4629

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Record 417 of 491

Title: Synergy of atom-probe structural data and quantum-mechanical calculations in a theory-guided design of extreme-stiffness superlattices containing metastable phases
Author(s): Friak, M (Friak, M.); Tytko, D (Tytko, D.); Holec, D (Holec, D.); Choi, PP (Choi, P-P); Eisenlohr, P (Eisenlohr, P.); Raabe, D (Raabe, D.); Neugebauer, J (Neugebauer, J.)
Source: NEW JOURNAL OF PHYSICS **Volume:** 17 **Article Number:** 093004 **DOI:** 10.1088/1367-2630/17/9/093004 **Published:** SEP 2 2015
Abstract: A theory-guided materials design of nano-scaled superlattices containing metastable phases is critically important for future development of advanced lamellar composites with application-dictated stiffness and hardness. Our study combining theoretical and experimental methods exemplifies the strength of this approach for the case of the elastic properties of AlN/CrN superlattices that were deposited by reactive radio-frequency magnetron sputtering with a bilayer period of 4 nm. Importantly, CrN stabilizes AlN in a metastable B1 (rock salt) cubic phase only in the form of a layer that is very thin, up to a few nanometers. Due to the fact that B1-AlN crystals do not exist as bulk materials, experimental data for this phase are not available. Therefore, quantum-mechanical calculations have been applied to simulate an AlN/CrN superlattice with a similar bilayer period. The ab initio predicted Young's modulus (428GPa) along the [001] direction is in excellent agreement with measured nano-indentation values (408 +/- 32 GPa). Aiming at a future rapid high-throughput materials design of superlattices, we have also tested predictions obtained within linear-elasticity continuum modeling using elastic properties of B1-CrN and B1-AlN phases as input. Using single-crystal elastic constants from ab initio calculations for both phases, we demonstrate the reliability of this approach to design nano-patterned coherent superlattices with unprecedented and potentially superior properties.
Accession Number: WOS:000367355100004
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Neugebauer, Joerg	K-2041-2015	0000-0002-7903-2472
Eisenlohr, Philip		0000-0002-8220-5995

ISSN: 1367-2630

Record 418 of 491

Title: Electronic and Chemical Properties of Donor, Acceptor Centers in Graphene
Author(s): Telychko, M (Telychko, Mykola); Mutombo, P (Mutombo, Pingo); Merino, P (Merino, Pablo); Hapala, P (Hapala, Prokop); Ondracek, M (Ondracek, Martin); Bocquet, FC (Bocquet, Francois C.); Sforzini, J (Sforzini, Jessica); Stetsovych, O (Stetsovych, Oleksandr); Vondracek, M (Vondracek, Martin); Jelinek, P (Jelinek, Pavel); Svec, M (Svec, Martin)
Source: ACS NANO **Volume:** 9 **Issue:** 9 **Pages:** 9180-9187 **DOI:** 10.1021/acsnano.5b03690 **Published:** SEP 2015
Abstract: Chemical doping is one of the most suitable ways of tuning the electronic properties of graphene and a promising candidate for a band gap opening. In this work we report a reliable and tunable method for preparation of high-quality boron and nitrogen co-doped graphene on silicon carbide substrate. We combine experimental (dAFM, STM, XPS, NEXAFS) and theoretical (total energy OFT and simulated STM) studies to analyze the structural, chemical, and electronic properties of the single-atom substitutional dopants in graphene. We show that chemical identification of boron and nitrogen substitutional defects can be achieved in the STM channel due to the quantum interference effect, arising due to the specific electronic structure of nitrogen dopant sites. Chemical reactivity of single boron and nitrogen dopants is analyzed using force distance spectroscopy by means of dAFM.
Accession Number: WOS:000361935800056
PubMed ID: 26256407
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Merino, Pablo	K-1392-2016	0000-0002-0267-4020
Stetsovych, Oleksandr	G-5742-2014	
Bocquet, Francois	B-7845-2010	0000-0002-9471-4439
Jelinek, Pavel	G-1542-2010	0000-0002-5645-8542
Svec, Martin	G-6645-2014	

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Record 419 of 491

Title: Exploring the electronic structure and optical properties of the quaternary selenide compound, Ba4Ga4SnSe12: For photovoltaic applications
Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz); Goumri-Said, S (Goumri-Said, Souraya)
Source: JOURNAL OF SOLID STATE CHEMISTRY **Volume:** 229 **Pages:** 260-265 **DOI:** 10.1016/j.jssc.2015.06.015 **Published:** SEP 2015
Abstract: Due to huge demand on discovering new materials for energy, we used first-principle calculations to explore the electronic structure and optical properties of a recent quaternary selenide, namely Ba4Ga4SnSe12. The electronic structure and the optical properties of Ba4Ga4SnSe12 were calculated through a reliable approach of Engle Vosko-GGA (EV-GGA). We found that Ba4Ga4SnSe12 has a direct band gap of 2.14 eV positioned at Gamma. Acquiring the fundamental characteristics of Ba4Ga4SnSe12, we studied the linear optical properties like dielectric function in the energy range of 0-14 eV. From the dielectric function we noticed a weak directional anisotropy for the two components. The absorption spectrum indicates the possibility of greater multiple direct and indirect inter-band transitions in the visible regions and shows similar behavior with experimental spectrum. Ba4Ga4SnSe12 can be used as shielding material from UV radiations. Present study predicts that the Ba4Ga4SnSe12 is promising for photovoltaic applications due to their high absorption of solar radiations and photoconductivity in the visible range. (C) 2015 Elsevier Inc. All rights reserved.
Accession Number: WOS:000358815100033
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Goumri-Said, Souraya	G-5318-2012	0000-0002-9333-7862
Azam, Sikander		0000-0001-5923-1127

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Record 420 of 491

Title: Motion planning with adaptive motion primitives for modular robots
Author(s): Vonasek, V (Vonasek, Vojtech); Saska, M (Saska, Martin); Kosnar, K (Kosnar, Karel); Preucil, L (Preucil, Libor)
Source: APPLIED SOFT COMPUTING **Volume:** 34 **Pages:** 678-692 **DOI:** 10.1016/j.asoc.2015.05.002 **Published:** SEP 2015
Abstract: This paper presents a novel motion planning algorithm for modular robots moving in environments with diverse terrain conditions. This requires the planner to generate a suitable control signal for all actuators, which can be computationally intensive. To decrease the complexity of the planning task, the concept of motion primitives is used. The motion primitives generate simple motions like 'crawl-forward' or 'turn-left' and the motion planner constructs a plan using these primitives. To preserve the efficiency and robustness of the planner on varying terrains, a novel schema called RRT-AMP (Rapidly Exploring Random Trees with Adaptive Motion Primitives) for adapting the motion primitives is introduced. The adaptation procedure is integrated into the planning process, which allows the planner simultaneously to adapt the primitives and to use them to obtain the final plan. Besides adaptation in changing environments, RRT-AMP can adapt motion primitives if some module fails. The methods is experimentally verified with robots of different morphologies to show its adaptation and planning abilities in complex environments. (C) 2015 Elsevier B.V. All rights reserved.
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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kosnar, Karel		0000-0002-6362-4254

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eISSN: 1872-9681

Record 421 of 491

Title: Vibrational Properties of the Phosphate Group Investigated by Molecular Dynamics and Density Functional Theory
Author(s): Andrushchenko, V (Andrushchenko, Valery); Benda, L (Benda, Ladislav); Pav, O (Pav, Ondrej); Dracinsky, M (Dracinsky, Martin); Bour, P (Bour, Petr)
Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 119 **Issue:** 33 **Pages:** 10682-10692 **DOI:** 10.1021/acs.jpcb.5b05124 **Published:** AUG 20 2015
Abstract: The phosphate group (PO2-) is an important building block occurring in Many components of living matter including nucleic acids. It provides distinct features in vibrational spectra and is useful as a local probe of NA conformation and interactions with the environment. For this purpose, it is desirable to explore in detail various factors influencing spectral shapes of characteristic phosphate vibrations. In the present study, effects of the solvent and conformational averaging are analyzed for simple model: molecules, dimethylphosphate, ethylmethylphosphate; and ethylmethylthiophosphate. Infrared absorption (IR) and Raman spectra were measured and calculated using a combination of molecular dynamics (MD) and density functional theory (DFT). To fully understand the link between the structure and the spectra, the solvent has to be explicitly included in the computational modeling. The results indicate that vibrational properties of the phosphate moiety are very sensitive to its conformation and interactions with the aqueous environment indeed. Polarizable continuum solvent models without explicit water molecules provided significantly worse agreement with the experiment. The combined MD/DFT approach captures well spectral Characteristics for the model systems and constitutes the most reliable basis for exploration of phosphate vibrational properties in biomolecular structural studies.
Accession Number: WOS:000360026400030
PubMed ID: 26193890
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dracinsky, Martin	B-5813-2013	0000-0002-4495-0070
Andrushchenko, Valery	G-7970-2014	0000-0002-4874-0548
Bour, Petr	G-5561-2014	
Benda, Ladislav	D-8918-2011	0000-0003-4716-569X

ISSN: 1520-6106

Record 422 of 491

Title: First-Principles Predictions of Vibrational Raman Optical Activity of Globular Proteins
Author(s): Kessler, J (Kessler, Jiri); Kapitan, J (Kapitan, Josef); Bour, P (Bour, Petr)
Source: JOURNAL OF PHYSICAL CHEMISTRY LETTERS **Volume:** 6 **Issue:** 16 **Pages:** 3314-3319 **DOI:** 10.1021/acs.jpclett.5b01500 **Published:** AUG 20 2015
Abstract: Computational methods based on the Schrodinger equation have been traditionally confined to rather small molecules. Using an automatic computational methodology, however, we obtained a stunning agreement between experimental and theoretical vibrational spectra of large globular proteins containing thousands of atoms as well. Principle atomic properties are obtained from small molecular fragments and combined with a minimal accuracy loss. This "first-principles" interpretation of the data reveals a wealth of information, such as nature of localized molecular motions as well as collective vibrational modes describing folding of larger protein parts. A new insight is provided to the origin of the chiroptical effects, and the theory lends the used spectroscopic techniques, unpolarized Raman scattering and vibrational Raman optical activity, immense potential to structural studies of biological systems.
Accession Number: WOS:000360027000014
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kessler, Jiri	G-2880-2012	0000-0001-6307-4339
Bour, Petr	G-5561-2014	

ISSN: 1948-7185

Record 423 of 491

Title: Facet-controlled phase separation in supersaturated Au-Ni nanoparticles upon shape equilibration
Author(s): Herz, A (Herz, A.); Friak, M (Friak, M.); Rossberg, D (Rossberg, D.); Hentschel, M (Hentschel, M.); Theska, F (Theska, F.); Wang, D (Wang, D.); Holec, D (Holec, D.); Sob, M (Sob, M.); Schneeweiss, O (Schneeweiss, O.); Schaaf, P (Schaaf, P.)
Source: APPLIED PHYSICS LETTERS **Volume:** 107 **Issue:** 7 **Article Number:** 073109 **DOI:** 10.1063/1.4928627 **Published:** AUG 17 2015
Abstract: Solid-state dewetting is used to fabricate supersaturated, submicron-sized Au-Ni solid solution particles out of thin Au/Ni bilayers by means of a rapid thermal annealing technique. Phase separation in such particles is studied with respect to their equilibrium crystal (or Wulff) shape by subsequent annealing at elevated temperature. It is found that {100} faceting planes of the equilibrated particles are enriched with Ni and {111} faces with Au. Both phases are considered by quantum-mechanical calculations in combination with an error-reduction scheme that was developed to compensate for a missing exchange-correlation potential that would reliably describe both Au and Ni. The observed phase configuration is then related to the minimization of strongly anisotropic elastic energies of Au- and Ni-rich phases and results in a rather unique nanoparticle composite state that is characterized by nearly uniform value of elastic response to epitaxial strains all over the faceted surface. The same conclusion is yielded also by evaluating bi-axial elastic moduli when employing interpolated experimental elastic constants. This work demonstrates a useful route for studying features of physical metallurgy at the mesoscale. (C) 2015 AIP Publishing LLC.
Accession Number: WOS:000360390500052
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Schaaf, Peter	B-4934-2009	0000-0002-8802-6621
Wang, Dong	G-1498-2011	0000-0001-5940-9538
Hentschel, Martin		0000-0002-5682-5154
Holec, David		0000-0002-3516-1061

ISSN: 0003-6951
eISSN: 1077-3118

Record 424 of 491

Title: Impact of the Extended 1,1'-Bipyridinium Structure on the Electron Transfer and pi-Dimer Formation. Spectroelectrochemical and Computational Study
Author(s): Tarabek, J (Tarabek, Jan); Kolivoska, V (Kolivoska, Viliam); Gal, M (Gal, Miroslav); Pospisil, L (Pospisil, Lubomir); Valasek, M (Valasek, Michal); Kaminsky, J (Kaminsky, Jakub); Hromadova, M (Hromadova, Magdalena)
Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 119 **Issue:** 32 **Pages:** 18056-18065 **DOI:** 10.1021/acs.jpcc.5b04388 **Published:** AUG 13 2015
Abstract: The electrochemical reduction of the extended 1,1'-bipyridinium dication was investigated in detail by means of semiquantitative in situ electron paramagnetic resonance (EPR), UV-vis-NIR spectroelectrochemistry, and density functional theory (DFT) calculations. It was found that in the extended 1,1'-bipyridinium cation radical the spin density is localized on one of the pyridinium centers, which is in contrast to charge delocalization within the 4,4'-bipyridinium radical cation reported in the literature. The charge and spin density separation in the extended 1,1'-bipyridinium cation radical leads to pi-dimer formation in a triplet electronic configuration.
Accession Number: WOS:000359683800007
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Tarabek, Jan	G-5319-2014	0000-0003-0116-3824
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022
Kolivoska, Viliam	G-7229-2014	
Valasek, Michal	C-7201-2015	0000-0001-9382-6327
Gal, Miroslav	A-8804-2018	0000-0002-5573-4226
Pospisil, Lubomir	F-5195-2014	
Hromadova, Magdalena	C-2369-2011	0000-0002-3138-6917

ISSN: 1932-7447

Record 425 of 491

Title: Probing Charges on the Atomic Scale by Means of Atomic Microscopy

Author(s): Albrecht, F (Albrecht, F.); Repp, J (Repp, J.); Fleischmann, M (Fleischmann, M.); Scheer, M (Scheer, M.); Ondracek, M (Ondracek, M.); Jelinek, P (Jelinek, P.)

Source: PHYSICAL REVIEW LETTERS **Volume:** 115 **Issue:** 7 **Article Number:** 076101 **DOI:** 10.1103/PhysRevLett.115.076101 **Published:** AUG 13 2015

Abstract: Kelvin probe force spectroscopy was used to characterize the charge distribution of individual molecules with polar bonds. Whereas this technique represents the charge distribution with moderate resolution for large tip-molecule separations, it fails for short distances. Here, we introduce a novel local force spectroscopy technique which allows one to better disentangle electrostatic from other contributions in the force signal. It enables one to obtain charge-related maps at even closer tip-sample distances, where the lateral resolution is further enhanced. This enhanced resolution allows one to resolve contrast variations along individual polar bonds.

Accession Number: WOS:000359437000013

PubMed ID: 26317733

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Jelinek, Pavel	G-1542-2010	0000-0002-5645-8542
Scheer, Manfred	J-3232-2016	0000-0003-2182-5020
Repp, Jascha	B-1843-2014	0000-0003-2883-7083

ISSN: 0031-9007

eISSN: 1079-7114

Record 426 of 491

Title: Force-Driven Single-Atom Manipulation on a Low-Reactive Si Surface for Tip Sharpening

Author(s): Berger, J (Berger, Jan); Spadafora, EJ (Spadafora, Evan J.); Mutombo, P (Mutombo, Pingo); Jelinek, P (Jelinek, Pavel); Svec, M (Svec, Martin)

Source: SMALL **Volume:** 11 **Issue:** 30 **Pages:** 3686-3693 **DOI:** 10.1002/smll.201500092 **Published:** AUG 12 2015

Abstract: A single atomic manipulation on the delta-doped B:Si(111)-()R30 degrees surface using a low temperature dynamic atomic force microscopy based on the Kolibri sensor is investigated. Through a controlled vertical displacement of the probe, a single Si adatom in order to open a vacancy is removed. It is shown that this process is completely reversible, by accurately placing a Si atom back into the vacancy site. In addition, density functional theory simulations are carried out to understand the underlying mechanism of the atomic manipulation in detail. This process also rearranges the atoms at the tip apex, which can be effectively sharpened in this way. Such sharper tips allow for a deeper look into the Si adatom vacancy site. Namely, high-resolution images of the vacancy showing subsurface Si dangling bond triplets, which surround the substitutional B dopant atom in the first bilayer, are achieved.

Accession Number: WOS:000359307700014

PubMed ID: 25940994

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Spadafora, Evan	A-2106-2011	0000-0002-1994-3709
Svec, Martin	G-6645-2014	
Jelinek, Pavel	G-1542-2010	0000-0002-5645-8542

ISSN: 1613-6810

eISSN: 1613-6829

Record 427 of 491

Title: From generalized stacking fault energies to dislocation properties: Five-energy-point approach and solid solution effects in magnesium

Author(s): Pei, ZR (Pei, Zongrui); Ma, DC (Ma, Duancheng); Friak, M (Friak, Martin); Svendsen, B (Svendsen, Bob); Raabe, D (Raabe, Dierk); Neugebauer, J (Neugebauer, Joerg)

Source: PHYSICAL REVIEW B **Volume:** 92 **Issue:** 6 **Article Number:** 064107 **DOI:** 10.1103/PhysRevB.92.064107 **Published:** AUG 11 2015

Abstract: Using ab initio calculations and symmetrized plane waves, we analyze the basal-plane generalized stacking fault energies in pure Mg and Mg-Y alloys and show that the knowledge of energies of only five specific points is sufficient to accurately predict the core structures and Peierls stresses of < a >-type edge dislocations in these alloys. Our five-point approach substantially reduces the computational cost related to the Peierls-Nabarro (PN) model and allows for a high-throughput application of the PN model to study Peierls stress changes in Mg upon alloying. We employ our approach to study Mg binary alloys containing nine rare-earth (RE) and 11 other solutes. Based on the Peierls stresses of these 20 Mg alloys calculated from the Peierls-Nabarro model, the solutes are divided into three groups: (i) the first group, consisting of Be, Zn, Tl, Tc, Os, Ru, Re, and Co, when added as solutes into Mg, lead to more compact dislocation core structures and larger Peierls stresses than found for pure Mg. (ii) Elements in the second group, including Ti, Nd, Lu, Zr, Hf, La, and Pr change the core widths and Peierls stresses moderately. (iii) The solutes in the third group containing Y, Er, Tm, Ho, and Sc extend the stacking fault width, and the resulting Peierls stresses are generally very low. Based on an error analysis, we conclude that the first group has a clear solute strengthening effect and the third group has a clear solute softening effect, while the effects of the elements in the second group are too small to be resolved by the present approach.

Accession Number: WOS:000359355000002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Neugebauer, Joerg	K-2041-2015	0000-0002-7903-2472
Raabe, Dierk	A-6470-2009	0000-0003-0194-6124
Svendsen, Bob	D-6311-2014	0000-0002-1519-9433
Ma, Duancheng	N-1231-2016	
Pei, Zongrui		0000-0003-0748-4629

ISSN: 1098-0121

eISSN: 1550-235X

Record 428 of 491

Title: Rotaxanes Capped with Host Molecules: Supramolecular Behavior of Adamantylated Bisimidazolium Salts Containing a Biphenyl Centerpiece

Author(s): Branna, P (Branna, Petra); Rouchal, M (Rouchal, Michal); Pruckova, Z (Pruckova, Zdenka); Dastychova, L (Dastychova, Lenka); Lenobel, R (Lenobel, Rene); Pospisil, T (Pospisil, Tomas); Malac, K (Malac, Kamil); Vicha, R (Vicha, Robert)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 21 **Issue:** 33 **Pages:** 11712-+ **DOI:** 10.1002/chem.201501353 **Published:** AUG 10 2015

Abstract: Bisimidazolium salts with one central biphenyl binding site and two terminal adamantyl binding sites form water-soluble binary or ternary aggregates with cucurbit[7]uril (CB7) and -cyclodextrin (-CD) with rotaxane and pseudorotaxane architectures. The observed arrangements result from cooperation of the supramolecular stopper binding strength and steric barriers against free slippage of the CB7 and -CD host molecules over the bisimidazolium guest axle.

Accession Number: WOS:000359084700002

PubMed ID: 26140503

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Rouchal, Michal	H-6380-2012	0000-0002-0117-4040
Vicha, Robert	H-6360-2012	
Dastychova, Lenka	O-2232-2016	0000-0003-3416-329X
Lenobel, Rene		0000-0001-7387-0056
Pospisil, Tomas		0000-0003-3634-828X
Pruckova, Zdenka		0000-0002-8327-6429

ISSN: 0947-6539
eISSN: 1521-3765

Record 429 of 491

Title: Surface-termination-dependent magnetism and strong perpendicular magnetocrystalline anisotropy of an FeRh(001) thin film
Author(s): Jekal, S (Jekal, Soyoung); Rhim, SH (Rhim, S. H.); Hong, SC (Hong, S. C.); Son, WJ (Son, Won-joon); Shick, AB (Shick, A. B.)
Source: PHYSICAL REVIEW B **Volume:** 92 **Issue:** 6 **Article Number:** 064410 **DOI:** 10.1103/PhysRevB.92.064410 **Published:** AUG 6 2015
Abstract: The magnetism of FeRh (001) films strongly depends on film thickness and surface terminations. While the magnetic ground state of bulk FeRh isG-type antiferromagnetism, the Rh-terminated films exhibit ferromagnetism with strong perpendicular magnetocrystalline anisotropy whose energy +2.1 meV/square is two orders of magnitude greater than bulk 3d conventional magnetic metals (square is the area of a two-dimensional unit cell). While the Goodenough-Kanamori-Anderson rule on the superexchange interaction is crucial in determining the magnetic ground phases of FeRh bulk and thin films, the magnetic phases are the results of interplay and competition between three mechanisms-the superexchange interaction, the Zener-type direct interaction, and energy gain by Rh magnetization.
Accession Number: WOS:000359046500007
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Shick, Alexander	C-1420-2013	0000-0003-2700-5517

ISSN: 1098-0121
eISSN: 1550-235X

Record 430 of 491

Title: Free motion around black holes with discs or rings: between integrability and chaos - IV
Author(s): Witzany, V (Witzany, V.); Semerak, O (Semerak, O.); Sukova, P (Sukova, P.)
Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY **Volume:** 451 **Issue:** 2 **Pages:** 1770-1794 **DOI:** 10.1093/mnras/stv1148 **Published:** AUG 1 2015
Abstract: The dynamical system studied in previous papers of this series, namely a bound time-like geodesic motion in the exact static and axially symmetric space-time of an (originally) Schwarzschild black hole surrounded by a thin disc or ring, is considered to test whether the often employed 'pseudo-Newtonian' approach (resorting to Newtonian dynamics in gravitational potentials modified to mimic the black hole field) can reproduce phase-space properties observed in the relativistic treatment. By plotting Poincare surfaces of section and using two recurrence methods for similar situations as in the relativistic case, we find similar tendencies in the evolution of the phase portrait with parameters (mainly with mass of the disc/ring and with energy of the orbiters), namely those characteristic to weakly non-integrable systems. More specifically, this is true for the Paczynski-Wiita and a newly suggested logarithmic potential, whereas the Nowak-Wagoner potential leads to a different picture. The potentials and the exact relativistic system clearly differ in delimitation of the phase-space domain accessible to a given set of particles, though this mainly affects the chaotic sea whereas not so much the occurrence and succession of discrete dynamical features (resonances). In the pseudo-Newtonian systems, the particular dynamical features generally occur for slightly smaller values of the perturbation parameters than in the relativistic system, so one may say that the pseudo-Newtonian systems are slightly more prone to instability. We also add remarks on numerics (a different code is used than in previous papers), on the resemblance of dependence of the dynamics on perturbing mass and on orbital energy, on the difference between the Newtonian and relativistic Bach-Weyl rings, and on the relation between Poincare sections and orbital shapes within the meridional plane.
Accession Number: WOS:000360830000050
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Semerak, Oldrich	C-2126-2017	0000-0002-1272-6779
Witzany, Vojtech		0000-0002-9209-5355
Sukova, Petra		0000-0002-4779-5635

ISSN: 0035-8711
eISSN: 1365-2966

Record 431 of 491

Title: Detection of Diverse Novel Bat Astrovirus Sequences in the Czech Republic
Author(s): Dufkova, L (Dufkova, Lucie); Strakova, P (Strakova, Petra); Sirmarova, J (Sirmarova, Jana); Salat, J (Salat, Jiri); Moutelikova, R (Moutelikova, Romana); Chrudimsky, T (Chrudimsky, Tomas); Bartonicka, T (Bartonicka, Tomas); Nowotny, N (Nowotny, Norbert); Ruzek, D (Ruzek, Daniel)
Source: VECTOR-BORNE AND ZOONOTIC DISEASES **Volume:** 15 **Issue:** 8 **Pages:** 518-521 **DOI:** 10.1089/vbz.2015.1813 **Published:** AUG 1 2015
Abstract: Astroviruses are a major cause of gastroenteritis in humans and animals. Recently, novel groups of astroviruses were identified in apparently healthy insectivorous bats. We report the detection of diverse novel astrovirus sequences in nine different European bat species: Eptesicus serotinus, Hypsugo savii, Myotis emarginatus, M. mystacinus, Nyctalus noctula, Pipistrellus nathusii or P. pygmaeus, P. pipistrellus, Vespertilio murinus, and Rhinolophus hipposideros. In six bat species, astrovirus sequences were detected for the first time. One astrovirus strain detected in R. hipposideros clustered phylogenetically with Chinese astrovirus strains originating from bats of the families Rhinolophidae and Hipposideridae. All other Czech astrovirus sequences from vesper bats formed, together with one Hungarian sequence, a separate monophyletic lineage within the bat astrovirus group. These findings provide new insights into the molecular epidemiology, ecology, and prevalence of astroviruses in European bat populations.
Accession Number: WOS:000359604300010
PubMed ID: 26273815
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ruzek, Daniel	G-9275-2014	
Strakova, Petra	S-8860-2016	0000-0002-3130-933X
Chrudimsky, Tomas	L-5628-2014	
Ruzek, Daniel		0000-0003-4655-2380

ISSN: 1530-3667
eISSN: 1557-7759

Record 432 of 491

Title: LazyFluids: Appearance Transfer for Fluid Animations
Author(s): Jamriska, O (Jamriska, Ondrej); Fiser, J (Fiser, Jakub); Asente, P (Asente, Paul); Lu, JW (Lu, Jingwan); Shechtman, E (Shechtman, Eli); Sykora, D (Sykora, Daniel)
Source: ACM TRANSACTIONS ON GRAPHICS **Volume:** 34 **Issue:** 4 **Article Number:** 92 **DOI:** 10.1145/2766983 **Published:** AUG 2015
Abstract: In this paper we present a novel approach to appearance transfer for fluid animations based on flow-guided texture synthesis. In contrast to common practice where pre-captured sets of fluid elements are combined in order to achieve desired motion and look, we bring the possibility of fine-tuning motion properties in advance using CG techniques, and then transferring the desired look from a selected appearance exemplar. We demonstrate that such a practical workflow cannot be simply implemented using current state-of-the-art techniques, analyze what the main obstacles are, and propose a solution to resolve them. In addition, we extend the algorithm to allow for synthesis with rich boundary effects and video exemplars. Finally, we present numerous results that demonstrate the versatility of the proposed approach.
Accession Number: WOS:000358786600058

Conference Title: ACM SIGGRAPH Conference
Conference Date: AUG 09-13, 2015
Conference Location: Los Angeles, CA
Conference Sponsors: ACM SIGGRAPH
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sykora, Daniel	C-3075-2014	0000-0002-6145-5151

ISSN: 0730-0301
eISSN: 1557-7368

Record 433 of 491

Title: Structural Changes in Ceramide Bilayers Rationalize Increased Permeation through Stratum Corneum Models with Shorter Acyl Tails
Author(s): Paloncyova, M (Paloncyova, Marketa); Vavrova, K (Vavrova, Katerina); Sovova, Z (Sovova, Zofie); DeVane, R (DeVane, Russell); Otyepka, M (Otyepka, Michal); Berka, K (Berka, Karel)
Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 119 **Issue:** 30 **Pages:** 9811-9819 **DOI:** 10.1021/acs.jpcb.5b05522 **Published:** JUL 30 2015
Abstract: Ceramides are indispensable constituents of the stratum corneum (SC), the uppermost impermeable layer of human skin. Ceramides with shorter (four- to eight-carbon acyl chains) fatty acid chains increase skin and model membrane permeability, while further shortening of the chain leads to increased resistance to penetration almost as good as that of ceramides from healthy skin (24 carbons long on average). Here we address the extent to which the atomistic CHARMM36 and coarse-grain MARTINI molecular dynamics (MD) simulations reflect the skin permeability data. As a result, we observed the same bell-shaped permeability trend for water that was observed in the skin and multilayer membrane experiments for model compounds We showed that the enhanced permeability of the short ceramides is mainly caused by the disturbance of their headgroup conformation because of their inability to accommodate the shorter lipid acyl chain into a typical hairpin conformation, Which further led to their destabilization and phase separation. As MD simulations described well delicate structural features of SC membranes, they seem to be suitable for further studies of the SC superstructure, including the development of skin penetration enhancers for transdermal drug delivery and skin toxicity risk assessment studies.
Accession Number: WOS:000359031400034
PubMed ID: 26151643
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Otyepka, Michal	D-1220-2017	0000-0002-1066-5677
Berka, Karel	E-2839-2010	0000-0001-9472-2589
Vavrova, Katerina	A-2895-2008	0000-0002-8502-4372
Otyepka, Michal	A-5922-2008	

ISSN: 1520-6106

Record 434 of 491

Title: Structure and Distribution of Cross-Links in Boron-Modified Phenol-Formaldehyde Resins Designed for Soft Magnetic Composites: A Multiple-Quantum B-11-B-11 MAS NMR Correlation Spectroscopy Study
Author(s): Kobera, L (Kobera, Libor); Czernek, J (Czernek, Jiri); Streckova, M (Streckova, Magda); Urbanova, M (Urbanova, Martina); Abbrent, S (Abbrent, Sabina); Brus, J (Brus, Jiri)
Source: MACROMOLECULES **Volume:** 48 **Issue:** 14 **Pages:** 4874-4881 **DOI:** 10.1021/acs.macromol.5b01037 **Published:** JUL 28 2015
Abstract: Despite the extensive use of boron-modified phenol-formaldehyde polymers as insulating materials in soft magnetic composites (SMCs), the structure and arrangement of the inorganic cross-linking units in these systems have not been fully elucidated. To clarify the structure, configuration, and distribution of the boron cross-links in these materials, phenol-formaldehyde resins modified by boric acid were synthesized and characterized using,advanced multiple-quantum B-11-B-11 MAS NMR correlation techniques combined with the quantum chemical geometry optimizations and the subsequent B-11 NMR chemical shielding calculations. The analyses of the resulting spectra revealed a well evolved (high-density) phenol-formaldehyde polymer network additionally strengthened by nitrogen and boron cross-links. The boron-based cross-links were attributed to monoester (ca. 10%) and diester (ca. 90%) complexes (six-membered spirocyclic borate anions) with strictly tetrahedral coordination (B-IV). During the thermal treatment, the monoester and diester borate complexes underwent additional transformation in which the spirocyclic borate anions were more tightly incorporated into the polymer matrix via additional N-type (amino) cross-links. A B-11-B-11 double-quantum correlation MAS NMR experiment revealed that the majority of the monoester and diester borate complexes (ca. 80%) were uniformly distributed within and effectively isolated by the polymer matrix, with an average B-11-B-11 interatomic distance greater than 6 angstrom. A non-negligible part of the spirocyclic borate anion complexes (ca. 20%), however, existed in pairs or small clusters in which the average B-11 center dot center dot center dot B-11 interatomic distance was less than 5.5 angstrom. In addition, the formation of homodimers (diester-diester) was' demonstrated to be preferred over the formation of heteroclusters (monoester-diester).
Accession Number: WOS:000358823300011
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kobera, Libor	G-5237-2014	0000-0002-8826-948X
Brus, Jiri	G-3459-2014	
Abbrent, Sabina	M-9812-2014	
Urbanova, Martina	G-9793-2014	0000-0003-1316-6395
Czernek, Jiri	H-6708-2014	
Brus, Jiri		0000-0003-2692-612X

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eISSN: 1520-5835

Record 435 of 491

Title: Centromeres Off the Hook: Massive Changes in Centromere Size and Structure Following Duplication of CenH3 Gene in Fabeae Species
Author(s): Neumann, P (Neumann, Pavel); Pavlikova, Z (Pavlikova, Zuzana); Koblizkova, A (Koblizkova, Andrea); Fukova, I (Fukova, Iva); Jedlickova, V (Jedlickova, Veronika); Novak, P (Novak, Petr); Macas, J (Macas, Jiri)
Source: MOLECULAR BIOLOGY AND EVOLUTION **Volume:** 32 **Issue:** 7 **Pages:** 1862-1879 **DOI:** 10.1093/molbev/msv070 **Published:** JUL 2015
Abstract: In most eukaryotes, centromere is determined by the presence of the centromere-specific histone variant CenH3. Two types of chromosome morphology are generally recognized with respect to centromere organization. Monocentric chromosomes possess a single CenH3-containing domain in primary constriction, whereas holocentric chromosomes lack the primary constriction and display dispersed distribution of CenH3. Recently, metapolycentric chromosomes have been reported in Pisum sativum, representing an intermediate type of centromere organization characterized by multiple CenH3-containing domains distributed across large parts of chromosomes that still form a single constriction. In this work, we show that this type of centromere is also found in other Pisum and closely related Lathyrus species, whereas Vicia and Lens genera, which belong to the same legume tribe Fabeae, possess only monocentric chromosomes. We observed extensive variability in the size of primary constriction and the arrangement of CenH3 domains both between and within individual Pisum and Lathyrus species, with no obvious correlation to genome or chromosome size. Search for CenH3 gene sequences revealed two paralogous variants, CenH3-1 and CenH3-2, which originated from a duplication event in the common ancestor of Fabeae species. The CenH3-1 gene was subsequently lost or silenced in the lineage leading to Vicia and Lens, whereas both genes are retained in Pisum and Lathyrus. Both of these genes appear to have evolved under purifying selection and produce functional CenH3 proteins which are fully colocalized. The findings described here provide the first evidence for a highly dynamic centromere structure within a group of closely related species, challenging previous concepts of centromere evolution.
Accession Number: WOS:000360585900016
PubMed ID: 25771197
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Fukova, Iva	G-9415-2014	0000-0002-2472-0665
Novak, Petr	A-3059-2013	0000-0002-5068-9681
Neumann, Pavel	H-7345-2013	0000-0001-6711-6639
Jedlickova, Veronika	I-5723-2014	
Macas, Jiri	G-8618-2014	0000-0003-0829-1570

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eISSN: 1537-1719

Record 436 of 491

Title: X-ray irradiation of the winds in binaries with massive components
Author(s): Krticka, J (Krticka, J.); Kubat, J (Kubat, J.); Krtickova, I (Krtickova, I.)
Source: ASTRONOMY & ASTROPHYSICS **Volume:** 579 **Article Number:** A111 **DOI:** 10.1051/0004-6361/201525637 **Published:** JUL 2015
Abstract: Context. Binaries with hot massive components are strong X-ray sources. Besides the intrinsic X-ray emission of individual binary members originating in their winds, X-ray emission stems from the accretion on the compact companion or from wind collision. Since hot star winds are driven by the light absorption in the lines of heavier elements, wind acceleration is sensitive to the ionization state. Therefore, the over-ionization induced by external X-ray source strongly influences the winds of individual components.
Aims. We studied the effect of external X-ray irradiation on hot star winds. Methods. We used our kinetic equilibrium (NLTE) wind models to estimate the influence of external X-ray ionization for different X-ray luminosities and source distances. The models are calculated for parameters typical of O stars.
Results. The influence of X-rays is given by the X-ray luminosity, by the optical depth between a given point and the X-ray source, and by a distance to the X-ray source. Therefore, the results can be interpreted in the diagrams of X-ray luminosity vs. the optical depth parameter. X-rays are negligible in binaries with low X-ray luminosities or at large distances from the X-ray source. The influence of X-rays is stronger for higher X-ray luminosities and in closer proximity of the X-ray source. There is a forbidden area with high X-ray luminosities and low optical depth parameters, where the X-ray ionization leads to wind inhibition. There is excellent agreement between the positions of observed stars in these diagrams and our predictions. All wind-powered high-mass X-ray binary primaries lie outside the forbidden area. Many of them lie close to the border of the forbidden area, indicating that their X-ray luminosities are self-regulated. We discuss the implications of our work for other binary types.
Conclusions. X-rays have a strong effect on the winds in binaries with hot components. The magnitude of the influence of X-rays can be estimated from the position of a star in the diagram of X-ray luminosity vs. the optical depth parameter.
Accession Number: WOS:000358877100123
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kubat, Jiri	G-9032-2014	0000-0003-4269-8278

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Record 437 of 491

Title: Prioritized Planning Algorithms for Trajectory Coordination of Multiple Mobile Robots
Author(s): Cap, M (Cap, Michal); Novak, P (Novak, Peter); Kleiner, A (Kleiner, Alexander); Selecky, M (Selecky, Martin)
Source: IEEE TRANSACTIONS ON AUTOMATION SCIENCE AND ENGINEERING **Volume:** 12 **Issue:** 3 **Pages:** 835-849 **DOI:** 10.1109/TASE.2015.2445780 **Published:** JUL 2015
Abstract: In autonomous multirobot systems one of the concerns is how to prevent collisions between the individual robots. One approach to this problem involves finding coordinated trajectories from start to destination for all the robots and then letting the robots follow the preplanned coordinated trajectories. A widely used practical method for finding such coordinated trajectories is "classical" prioritized planning, where robots plan sequentially one after another. This method has been shown to be effective in practice, but it is incomplete (i.e., there are solvable problem instances that the algorithm fails to solve) and it has not yet been formally analyzed under what circumstances is the method guaranteed to succeed. Further, prioritized planning is a centralized algorithm, which makes the method unsuitable for decentralized multirobot systems.
The contributions of this paper are: a) an adapted version of classical prioritized planning called revised prioritized planning with a formal characterization of a class of instances that are provably solvable by this algorithm and b) an asynchronous decentralized variant of both classical and revised prioritized planning together with a formal analysis showing that the algorithm terminates and inherits completeness properties from its centralized counterpart.
The experimental evaluation performed in simulation on real-world indoor maps shows that: a) the revised version of prioritized planning reliably solves a wide class of instances on which both classical prioritized planning and popular reactive technique ORCA fail and b) the asynchronous decentralized implementation of classical and revised prioritized planning finds solution in large multirobot teams up to 2x-faster than the previously proposed synchronized decentralized approach.
Note to Practitioners-Consider a large warehouse in which the goods are stored and retrieved by autonomous mobile robots. One way to deal with possible collisions between the robots is to ignore interactions between the vehicles during the route planning for each robot and handle the conflicts only during the route execution. However, such an approach is prone to deadlocks, i.e., to situations during which some of the robots mutually block each other, cannot proceed and fail to complete their transportation task. An alternative approach would involve planning collision-free routes for each robot before the robots start executing them. However, the current methods that guarantee ability to find a solution to any such coordination problem are not applicable in practice due to their high computational complexity. Instead, a simple and computationally efficient approach in which robots plan their routes sequentially one after another (classical prioritized planning) is often used for finding coordinated trajectories even though the algorithm is known to fail on many dense problem instances. In this paper, we show that a simple adaptation of this classical algorithm called revised prioritized planning is guaranteed to find collision-free trajectories for a well-defined class of practical problems. In particular, if the system resembles human-made transport infrastructures by requiring that the start and destination position of each vehicle must never obstruct other vehicles from moving, then the proposed approach is guaranteed to provide a solution. For instance, in our warehouse multirobot system example, the collision-free routes can be efficiently computed by the revised prioritized planning approach. This paper formally characterizes the problem instances for which the method is guaranteed to succeed.
Further, we propose a new asynchronous decentralized adaptation of both classical and revised prioritized algorithm that can be used in multirobot systems without a central solver. This technique can be used to find coordinated trajectories just by running a simple asynchronous negotiation protocol between the individual robots. This paper provides an analysis showing that the asynchronous decentralized implementations of classical and revised prioritized planning exhibit desirable theoretical properties and an experimental comparison of performance of different variations of centralized and decentralized prioritized planning algorithms.
Accession Number: WOS:000358585200007
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Record 438 of 491

Title: Evaluation of Selected Classical Force Fields for Alchemical Binding Free Energy Calculations of Protein-Carbohydrate Complexes
Author(s): Mishra, SK (Mishra, Sushil K.); Calabro, G (Calabro, Gaetano); Loeffler, HH (Loeffler, Hannes H.); Michel, J (Michel, Julien); Koca, J (Koca, Jaroslav)
Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 11 **Issue:** 7 **Pages:** 3333-3345 **DOI:** 10.1021/acs.jctc.5b00159 **Published:** JUL 2015
Abstract: Protein carbohydrate recognition is crucial in many vital biological processes including host-pathogen recognition, cell-signaling, and catalysis. Accordingly, computational prediction of protein-carbohydrate binding free energies is of enormous interest for drug design. However, the accuracy of current force fields (FFs) for predicting binding free energies of protein-carbohydrate complexes is not well understood owing to technical challenges such as the highly polar nature of the complexes, anomerization, and conformational flexibility of carbohydrates. The present study evaluated the performance of alchemical predictions of binding free energies with the GAFF1.7/AM1-BCC and GLYCAMO6j force fields for modeling protein carbohydrate complexes. Mean unsigned errors of 1.1 +/- 0.06 (GLYCAMO6j) and 2.6 +/- 0.08 (GAFF1.7/AM1-BCC) kcal.mol(-1) are achieved for a large data set of monosaccharide ligands for Ralstonia solanacearum lectin (RSL). The level of accuracy provided by GLYCAMO6j is sufficient to discriminate potent, moderate, and weak binders, a goal that has been difficult to achieve through other scoring approaches. Accordingly, the protocols presented here could find useful applications in carbohydrate-based drug and vaccine developments.
Accession Number: WOS:000358104800042
PubMed ID: 26575767
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Mishra, Sushil	O-4779-2014	0000-0002-3080-9754

ISSN: 1549-9618
eISSN: 1549-9626

Record 439 of 491

Title: Dependence of structure and properties of hard nanocrystalline conductive films MBCN (M = Ti, Zr, Hf) on the choice of metal element
Author(s): Houska, J (Houska, J.); Kohout, J (Kohout, J.); Mares, P (Mares, P.); Cerstvy, R (Cerstvy, R.); Vlcek, J (Vlcek, J.)
Source: THIN SOLID FILMS **Volume:** 586 **Pages:** 22-27 **DOI:** 10.1016/j.tsf.2015.04.023 **Published:** JUL 1 2015
Abstract: The paper deals with hard nanocrystalline conductive films MBCN(M = Ti, Zr, Hf) prepared by pulsed dc reactive magnetron sputtering. We focus on the effect of the choice of metal element (at fixed contents of the non-metal elements and fixed deposition parameters) on material structure and properties. We find that the transition from Ti through Zr to Hf leads to an increasing preference to form stable MBxCyN1-x-y solid solutions, and (consequently) to more pronounced crystallinity and texture. These results are compared with and explained by abinitio calculations. At a low N content the transition from X-ray amorphous TiBCN to truly nanocrystalline or even nanocomposite ZrBCN and HfBCN leads to increased hardness (from 21 to 33-37 GPa), increased hardness to effective Young's modulus ratio (from 0.098 to 0.132-0.133) and increased elastic recovery (from 67 to 82-85%). At a medium N content the transition from TiBCN (which is homogenous) to ZrBCN and HfBCN (where small conductive nanocrystals are separated by an insulating amorphous phase) dramatically increases the electrical resistivity (from the order of 10(-6) to the order of 10(3)-10(6) Omega m). The results are important for the design of future hard and electrically conductive protective coatings with a high thermal stability. (C) 2015 Elsevier B.V. All rights reserved.
Accession Number: WOS:000353984000004
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cerstvy, Radomir	C-3767-2016	0000-0001-8507-6642
Vlcek, Jaroslav	B-9259-2016	0000-0003-2627-2074
Houska, Jiri	B-9616-2016	0000-0002-4809-4128
Kohout, Jiri	N-8106-2016	0000-0002-5614-2126

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Record 440 of 491

Title: Hot electron refluxing in the short intense laser pulse interactions with solid targets and its influence on K-alpha radiation
Author(s): Horny, V (Horny, Vojtech); Klimo, O (Klimo, Ondrej)
Source: NUKLEONIKA **Volume:** 60 **Issue:** 2 **Pages:** 233-237 **DOI:** 10.1515/nuka-2015-0045 **Published:** JUN 2015
Abstract: Fast electrons created as a result of the laser beam interaction with a solid target penetrate into the target material and initialize processes leading to the generation of the characteristic X-ray K-alpha radiation. Due to the strong electric field induced at the rear side of a thin target the transmitted electrons are redirected back into the target. These refluxing electrons increase the K-alpha radiation yield, as well as the duration of the X-ray pulse and the size of the radiation emitting area. A model describing the electron refluxing was verified via particle-in-cell simulations for non-relativistic electron energies. Using this model it was confirmed that the effect of the electron refluxing on the generated X-ray radiation depends on the target thickness and the target material. A considarable increase of the number of the emitted K-alpha photons is observed especially for thin targets made of low-Z materials, and for higher hot electron temperatures.
Accession Number: WOS:000359955100007
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Klimo, Ondrej	B-2196-2010	0000-0002-0565-2409
Horny, Vojtech		0000-0002-4510-3770

ISSN: 0029-5922
eISSN: 1508-5791

Record 441 of 491

Title: Reaction Diffusion Voronoi Diagrams: From Sensors Data to Computing
Author(s): Vazquez-Otero, A (Vazquez-Otero, Alejandro); Faigl, J (Faigl, Jan); Dormido, R (Dormido, Raquel); Duro, N (Duro, Natividad)
Source: SENSORS **Volume:** 15 **Issue:** 6 **Pages:** 12736-12764 **DOI:** 10.3390/s150612736 **Published:** JUN 2015
Abstract: In this paper, a new method to solve computational problems using reaction diffusion (RD) systems is presented. The novelty relies on the use of a model configuration that tailors its spatiotemporal dynamics to develop Voronoi diagrams (VD) as a part of the system's natural evolution. The proposed framework is deployed in a solution of related robotic problems, where the generalized VD are used to identify topological places in a grid map of the environment that is created from sensor measurements. The ability of the RD-based computation to integrate external information, like a grid map representing the environment in the model computational grid, permits a direct integration of sensor data into the model dynamics. The experimental results indicate that this method exhibits significantly less sensitivity to noisy data than the standard algorithms for determining VD in a grid. In addition, previous drawbacks of the computational algorithms based on RD models, like the generation of volatile solutions by means of excitable waves, are now overcome by final stable states.
Accession Number: WOS:000357869200034
PubMed ID: 26035349
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Faigl, Jan	E-8685-2013	0000-0002-6193-0792
Dormido, Raquel	K-8647-2014	0000-0003-1175-5065
DURO, NATIVIDAD	K-8117-2014	0000-0001-9837-5967

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Record 442 of 491

Title: ASSEMBLING THE CHALLENGING PUZZLE OF ALGAL BIODIVERSITY: SPECIES DELIMITATION WITHIN THE GENUS ASTEROCHLORIS (TREBOUXIOPHYCEAE, CHLOROPHYTA)
Author(s): Skaloud, P (Skaloud, Pavel); Steinova, J (Steinova, Jana); Ridka, T (Ridka, Tereza); Vancurova, L (Vancurova, Lucie); Peksa, O (Peksa, Ondrej)
Source: JOURNAL OF PHYCOLOGY **Volume:** 51 **Issue:** 3 **Pages:** 507-527 **DOI:** 10.1111/jpy.12295 **Published:** JUN 2015
Abstract: The genus Asterochloris represents one of the most common, widespread, and diverse taxa of lichen photobionts. In this report, we describe and characterize six new species (A. echinata, A. friedlii, A. gaertneri, A. leprarii, A. lobophora, and A. woessiae) that were identified during our recent investigation of photobiont diversity. We found that the species differed genetically, morphologically, ecologically, and with respect to their mycobiont partners. Statistical analyses revealed significant morphological differentiation of all six newly described species, as well as their separation from previously described Asterochloris species. Chloroplast morphology represented the best morphological marker for species delineation. In fact, each species can be recognized by the dominance and unique assemblage of particular chloroplast types. Although genetically well recognized by rapidly evolving internal transcribed spacer rDNA and actin intron markers, all 13 investigated Asterochloris species shared identical small subunit rDNA sequences. We therefore demonstrated that morphologically and ecologically diverse species can frequently be grouped into a single taxonomic unit in whole-transcriptome sequencing studies, considerably affecting the resulting estimates of species diversity. Finally, we demonstrated the presence of isogamous sexual reproduction in Asterochloris, disputing the current symbiotic dogma of the loss of sexual reproduction in algal symbionts.
Accession Number: WOS:000356627000010
PubMed ID: 26986666
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vancurova, Lucie	I-5923-2016	0000-0002-1370-1020
Skaloud, Pavel	F-3103-2011	0000-0003-1201-3290

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Record 443 of 491

Title: A first principles study of electronic and optical properties of the polar quaternary chalcogenides beta-A(2)Hg(3)Ge(2)S(8)(A=K and Rb)
Author(s): Azam, S (Azam, Sikander); Khan, SA (Khan, Saleem Ayaz)
Source: MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING **Volume:** 34 **Pages:** 250-259 **DOI:** 10.1016/j.mssp.2015.02.042 **Published:** JUN 2015
Abstract: The beta-A(2)Hg(3)Ge(2)S(8) (A=K and Rb) materials have a unique structure, possessing the high infrared transmission. More studies on beta-A(2)Hg(3)Ge(2)S(8) (A=K and Rb) are significant to investigate the probability of using these materials for optoelectronic devices. This work presents the results dealing with electronic and optical properties of beta-A(2)Hg(3)Ge(2)S(8) (A=K and Rb) obtained from first-principles calculations. We used the full potential linear augmented plane wave (FPLAPW) scheme, in the framework of DFT with modified Becke Johnson approximation (mBJ). We present the band structure, density of states (DOS), and electronic charge density. In addition, the band structure calculation suggests that the beta-A(2)Hg(3)Ge(2)S(8) (A=K and Rb) are semiconductors with indirect band gaps of 2.497 and 2.481 eV for beta-K2Hg3Ge2S8 and beta-Rb2Hg3Ge2S8 compounds, which is in excellent agreement with the estimated value of 2.7 eV for beta-K2Hg3Ge2S8. An exhaustive study of the electronic density of states and the electronic charge density redistribution reveals the covalent bonding characteristics between Hg, Ge and S atoms.
To get the fundamental characteristics of these two compounds, we have probe their linear optical properties such as the dynamic dielectric function, energy loss function, reflectivity, refractive index and absorption coefficients, In the energy range of 0-15 eV. From the dynamic dielectric constant, the structural anisotropy is clearly observed.
Optical response study recommends that the imaginary part of dielectric function spectra is appropriated for to be the interband transition. (C) 2015 Elsevier Ltd. All rights reserved.
Accession Number: WOS:000353844500036
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Azam, Sikander		0000-0001-5923-1127

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eISSN: 1873-4081

Record 444 of 491

Title: High-level motion planning for CPG-driven modular robots
Author(s): Vonasek, V (Vonasek, Vojtech); Saska, M (Saska, Martin); Winkler, L (Winkler, Lutz); Preucil, L (Preucil, Libor)
Source: ROBOTICS AND AUTONOMOUS SYSTEMS **Volume:** 68 **Pages:** 116-128 **DOI:** 10.1016/j.robot.2015.01.006 **Published:** JUN 2015
Abstract: Modular robots may become candidates for search and rescue operations or even for future space missions, as they can change their structure to adapt to terrain conditions and to better fulfill a given task. A core problem in such missions is the ability to visit distant places in rough terrain. Traditionally, the motion of modular robots is modeled using locomotion generators that can provide various gaits, e.g. crawling or walking. However, pure locomotion generation cannot ensure that desired places in a complex environment with obstacles will in fact be reached. These cases require several locomotion generators providing motion primitives that are switched using a planning process that takes the obstacles into account. In this paper, we present a novel motion planning method for modular robots equipped with elementary motion primitives. The utilization of primitives significantly reduces the complexity of the motion planning which enables plans to be created for robots of arbitrary shapes. The primitives used here do not need to cope with environmental changes, which can therefore be realized using simple locomotion generators that are scalable, i.e., the primitives can provide motion for robots with many modules. As the motion primitives are realized using locomotion generators, no reconfiguration is required and the proposed approach can thus be used even for modular robots without self-reconfiguration capabilities. The performance of the proposed algorithm has been experimentally verified in various environments, in physical simulations and also in hardware experiments. (C) 2015 Elsevier B.V. All rights reserved.
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Record 445 of 491

Title: Determination of Absolute Configuration in Chiral Solvents with Nuclear Magnetic Resonance. A Combined Molecular Dynamics/Quantum Chemical Study
Author(s): Kessler, J (Kessler, Jiri); Dracinsky, M (Dracinsky, Martin); Bour, P (Bour, Petr)
Source: JOURNAL OF PHYSICAL CHEMISTRY A **Volume:** 119 **Issue:** 21 **Special Issue:** SI **Pages:** 5260-5268 **DOI:** 10.1021/jp509988e **Published:** MAY 28 2015
Abstract: Nuclear magnetic resonance (NMR) spectroscopy is omnipresent in :chemical analysis. However, chirality of a molecule can only be detected indirectly by NMR, e.g., by monitoring its interaction with another chiral object. In the present study, we investigate the spectroscopic behavior of chiral molecules placed into a chiral solvent. In this case, the solvent solute interaction is much weaker, but the application range of such NMR. analysis is wider than for,a specific chemical shift agent. Two alcohols and an amine were used as model systems, and differences in NMR chemical shifts dependent on the solute solvent chirality combination were experimentally detected. Combined quantum mechanic/molecular mechanic (QM/MM) computations were applied to reveal the underlying solute solvent interactions. NMR. shielding was calculated using the density functional theory (DFT). While the experimental observations could not be reproduced quantitatively, the modeling provided a qualitative agreement and detailed insight into the essence of solvent solute chiral interactions. The potentials of mean force (PMF) obtained using molecular dynamics (MD) and:. the weighted histogram analysis method (WHAM) indicate that the chiral interaction brings about differences in conformer ratios, which are to a large extent responsible for the NMR Shifts. The MD results also predicted slight changes in the solvent Structure, including the radial distribution function (RDF), to depend on the solvent/solute chirality combination. Apart from the conformer distribution, an effective average solvent electrostatic field was tested as another major factor contributing to the chiral NMR effect. The possibility to,simulate spectral effects of chiral solvents from the first-principles opens up the way to NMR spectroscopic determination of the absolute configuration for a larger scale of compounds, including those not forming specific complexes.
Accession Number: WOS:000355495100024
PubMed ID: 25411905
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dracinsky, Martin	B-5813-2013	0000-0002-4495-0070
Bour, Petr	G-5561-2014	
Kessler, Jiri	G-2880-2012	0000-0001-6307-4339

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Record 446 of 491

Title: Genetic analysis of clinical mastitis data for Holstein cattle in the Czech Republic
Author(s): Zavadilova, L (Zavadilova, L.); Stipkova, M (Stipkova, M.); Sebkova, N (Sebkova, N.); Svitakova, A (Svitakova, A.)
Source: ARCHIV FUR TIERZUCHT-ARCHIVES OF ANIMAL BREEDING **Volume:** 58 **Pages:** 199-204 **DOI:** 10.5194/aab-58-199-2015 **Published:** MAY 21 2015
Abstract: Cases of mastitis were recorded from 22 812 lactations of 10 294 cows on seven farms in the Czech Republic from 2000 to 2012. The per cow number of clinical mastitis (CM) cases per lactation (CM1), number of days of CM per lactation (CM2), and CM considered as an all-or-none trait (CM3) with values of 0 (no CM case) or 1 (at least 1 CM case) were analyzed with linear animal models. Bivariate linear animal models were used for estimation of genetic correlations between CM traits and average lactation somatic cell score (SCS305), average 305-day milk (MY305), fat (FY305) and protein (PY305) yield, and interval between calving and first insemination (INT) and days open (DO). Factors included in the model of choice were parity, herd effect, year of calving, calving season, permanent environmental effect of the cow, and additive genetic effect of the cow. Estimated heritabilities for CM traits were in the range of 0.09 to 0.10. Genetic correlations of SCS305 with CM traits 1, 2, and 3 were 0.22 +/- 0.062, 0.23 +/- 0.064, and 0.29 +/- 0.086, respectively; those of MY305 with the three CM traits were 0.80 +/- 0.037, 0.79 +/- 0.040, and 0.83 +/- 0.038, respectively; those of INT with the three CM traits were 0.19 +/- 0.087, 0.17 +/- 0.089, and 0.26 +/- 0.091, respectively; and those of DO with the three CM traits were 0.28 +/- 0.089, 0.22 +/- 0.091, and 0.27 +/- 0.091, respectively. Knowledge of genetic parameters of mastitis incidence and assessment of the economic importance of the disease is necessary to design breeding programs to improve udder health.
Accession Number: WOS:000357116000001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Zavadilovi, Ludmila	E-2121-2012	0000-0002-7124-2491
Sebkova, Natasa	B-6908-2015	0000-0002-0839-5620

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Record 447 of 491

Title: Molecular simulations of hevein/(GlcNAc)(3) complex with weakened OH/O and CH/pi hydrogen bonds: implications for their role in complex stabilization

Author(s): Mareska, V (Mareska, Vaclav); Tvaroska, I (Tvaroska, Igor); Kralova, B (Kralova, Blanka); Spiwok, V (Spiwok, Vojtech)

Source: CARBOHYDRATE RESEARCH **Volume:** 408 **Pages:** 1-7 **DOI:** 10.1016/j.carres.2015.02.012 **Published:** MAY 18 2015

Abstract: Carbohydrate-protein complexes are often characterized by interactions via aromatic amino acid residues. Several mechanisms have been proposed to explain these stacking-like interactions between pyranose sugars and aromatic moieties. The physical basis of these interactions is being explained as either dispersion CH/pi or hydrophobic. In order to elucidate the nature of these interactions, we performed a series of molecular dynamics simulation of hevein domain (HEV32) in complex with (beta-D-GlcNAc)(3). Selected OH/O and CH/pi hydrogen bonds involved in carbohydrate recognition were artificially weakened in 100 ns molecular dynamics simulations. Separate weakening of either OH/O or CH/pi hydrogen bonds was not sufficient to destabilize the complex. This indicates that other effects, not solely CH/pi dispersion interactions, contribute significantly to the stability of the complex. Significant destabilization of complexes was reached only by simultaneous weakening of OH/O and CH/pi hydrogen bonds. This also shows that classical hydrogen bonds and CH/pi interactions are working in concert to stabilize this carbohydrateeprotein test case. (C) 2015 Elsevier Ltd. All rights reserved.

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PubMed ID: 25816996

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Spiwok, Vojtech	A-7747-2008	0000-0001-8108-2033

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Record 448 of 491

Title: Evidence for precursor superconducting pairing above T-c in underdoped cuprates from an analysis of the in-plane infrared response

Author(s): Sopik, B (Sopik, B.); Chaloupka, J (Chaloupka, J.); Dubroka, A (Dubroka, A.); Bernhard, C (Bernhard, C.); Munzar, D (Munzar, D.)

Source: NEW JOURNAL OF PHYSICS **Volume:** 17 **Article Number:** 053022 **DOI:** 10.1088/1367-2630/17/5/053022 **Published:** MAY 15 2015

Abstract: We performed calculations of the in-plane infrared response of underdoped cuprate superconductors to clarify the origin of a characteristic dip feature which occurs in the published experimental spectra of the real part of the in-plane conductivity below an onset temperature T-ons considerably higher than T-c. We provide several arguments, based on a detailed comparison of our results with the published experimental data, confirming that the dip feature and the related features of the memory function M(omega)= M1(omega)+ iM2(omega)(a peak in M1 and a kink in M2) are due to superconducting pairing correlations that develop below T-ons. In particular, we show that (i) the dip feature, the peak and the kink of the low-temperature experimental data can be almost quantitatively reproduced by calculations based on a model of a d-wave superconductor. The formation of the dip feature in the experimental data below T-ons is shown to be analogous to the one occurring in the model spetra below T-c. (ii) Calculations based on simple models, for which the dip in the temperature range from T-c to T-ons is unrelated to superconducting pairing, predict a shift of the onset of the dip at the high-energy side upon entering the superconducting state, that is not observed in the experimental data; (iii) the conductivity data in conjunction with the recent photoemission data (Reber et al 2012 Nat. Phys. 8 606, Reber et al 2013 Phys. Rev. B 87 060506) imply the persistence of the coherence factor characteristic of superconducting pairing correlations in a range of temperatures above T-c.

Accession Number: WOS:000355279800003

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Chaloupka, Jiri	I-3636-2014	

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Record 449 of 491

Title: Insight into the Mechanism of the Thermal Reduction of Graphite Oxide: Deuterium-Labeled Graphite Oxide Is the Key

Author(s): Sofer, Z (Sofer, Zdenek); Jankovsky, O (Jankovsky, Ondrej); Simek, P (Simek, Petr); Sedmidubsky, D (Sedmidubsky, David); Sturala, J (Sturala, Jiri); Kosina, J (Kosina, Jiri); Miksova, R (Miksova, Romana); Mackova, A (Mackova, Anna); Mikulics, M (Mikulics, Martin); Pumera, M (Pumera, Martin)

Source: ACS NANO **Volume:** 9 **Issue:** 5 **Pages:** 5478-5485 **DOI:** 10.1021/acsnano.5b01463 **Published:** MAY 2015

Abstract: For the past decade, researchers have been trying to understand the mechanism of the thermal reduction of graphite oxide. Because deuterium is widely used as a marker in various organic reactions, we wondered if deuterium-labeled graphite oxide could be the key to fully understand this mechanism. Graphite oxides were prepared by the Hofmann, Hummers, Staudenmaier, and Brodie methods, and a deuterium-labeled analogue was synthesized by the Hofmann method. All graphite oxides were analyzed not only using the traditional techniques but also by gas chromatography-mass spectrometry (GC-MS) during exfoliation in hydrogen and nitrogen atmospheres. GC-MS enabled us to compare differences between the chemical compositions of the organic exfoliation products formed during the thermal reduction of these graphite oxides. Nuclear analytical methods (Rutherford backscattering spectroscopy, elastic recoil detection analysis) were used to calculate the concentrations of light elements, including the ratio of hydrogen to deuterium. Combining all of these results we were able to determine graphite oxide's thermal reduction mechanism. Carbon dioxide, carbon monoxide, and water are formed from the thermal reduction of graphite oxide. This process is also accompanied by various radical reactions that lead to the formation of a large amount of carcinogenic volatile organic compounds, and this will have major safety implications for the mass production of graphene.

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PubMed ID: 25894311

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Pumera, Martin	F-2724-2010	0000-0001-5846-2951
Sturala, Jiri	A-1253-2013	
Sedmidubsky, David	K-3874-2015	0000-0003-3191-8781
Miksova, Romana	G-9867-2014	
Sturala, Jiri	G-8229-2017	0000-0002-8113-0709
Sofer, Zdenek	A-9690-2010	0000-0002-1391-4448
Mackova, Anna	G-8536-2014	

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Record 450 of 491

Title: Transfer of Frequency-Dependent Polarizabilities: A Tool To Simulate Absorption and Circular Dichroism Molecular Spectra

Author(s): Kessler, J (Kessler, Jiri); Bour, P (Bour, Petr)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 11 **Issue:** 5 **Pages:** 2210-2220 **DOI:** 10.1021/acs.jctc.5b00136 **Published:** MAY 2015

Abstract: Absorption and circular dichroism spectra reveal important information about molecular geometry and electronic structure. For large molecules, however, spectral shapes cannot be computed directly. In the past, transition dipole coupling (TDC) and related theories were proposed as simplified ways of calculating the spectral responses of large systems. In the present study, an alternative approach better reflecting the chemical structure is explored. It is based on the transfer of complex frequency-dependent polarizabilities (TFDP) of molecular fragments. The electric dipoleelectric dipole, electric dipoleelectric quadrupole, and electric dipolemagnetic dipole polarizabilities are obtained separately for individual chromophores and then transferred to a larger system composed of them. Time-dependent density functional theory and the sum over states methodology were employed to obtain the polarizability tensors of N-methylacetamide, and porphyrin molecules were chosen for a numerical test. The TFDP fails for charge-transfer states and close chromophores; otherwise, the results suggest that this method is capable of reproducing the spectra of large systems of biochemical relevance. At the same time, it is sufficiently flexible to account for a wide range of transition energies and environmental factors instrumental in the modeling of chromophore properties. The TFDP approach also removes the

need for diagonalization in TDC, making computations of larger molecular systems more time-efficient.

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PubMed ID: 26574421

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kessler, Jiri	G-2880-2012	0000-0001-6307-4339
Bour, Petr	G-5561-2014	

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Page 10 (Records 451 -- 491)
◀ [1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10] ▶

Print

Record 451 of 491

Title: Theoretical investigation of electronic structure and optical response in relation to the transport properties of Ga1-xInxN (x=0, 0.25, 0.50, 0.75)

Author(s): Shah, FA (Shah, Fahad Ali); Khan, SA (Khan, Saleem Ayaz); Arif, S (Arif, Suneela); Azam, S (Azam, Sikander); Khenata, R (Khenata, R.); Bin Omran, S (Bin Omran, S.)

Source: CURRENT APPLIED PHYSICS **Volume:** 15 **Issue:** 5 **Pages:** 608-616 **DOI:** 10.1016/j.cap.2015.02.014 **Published:** MAY 2015

Abstract: The state-of-the-art all-electron FLPAW method and the BoltzTrap software package based on semi-classical theory were adopted to explore the electronic structure and the optical and thermoelectric properties of Ga1-xInxN. Ga1-xInxN is predicted to be a direct band gap material for all values of x. Moreover, the band gap varies between 2.99 eV and 1.95 eV as x changes. Optical parameters such as the dielectric constant, absorption coefficient, reflectivity and refractive index are calculated and discussed in detail. The doping of In plays an important role in the modulation of the optical constants. The static dielectric constant epsilon(0) of Ga1-xInxN was calculated as 3.95, 3.99, 3.99 and 4.03 at x = 0.00, 0.25, 0.50 and 0.75, respectively. The static refractive index is 2.0 for pure Ga1-xInxN at x = 0.00. The thermal properties varied greatly as x fluctuated. The ternary alloy has large values for the Seebeck coefficient and figure of merit at high temperatures and is thus suitable for thermoelectric applications. Pure Ga1-xInxN at x = 0 exhibited ZT = 0.80 at room temperature, and at higher temperatures, the thermal conductivity decreased with increased In doping. (C) 2015 Elsevier B.V. All rights reserved.

Accession Number: WOS:000352280000008

Author Identifiers:

Author	ResearcherID Number	ORCID Number
BINOMRAN, SAAD	N-7968-2016	0000-0001-6097-2344
Azam, Sikander		0000-0001-5923-1127

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Record 452 of 491

Title: Latent semantics in Named Entity Recognition

Author(s): Konkol, M (Konkol, Michal); Brychcin, T (Brychcin, Tomas); Konopik, M (Konopik, Miloslav)

Source: EXPERT SYSTEMS WITH APPLICATIONS **Volume:** 42 **Issue:** 7 **Pages:** 3470-3479 **DOI:** 10.1016/j.eswa.2014.12.015 **Published:** MAY 1 2015

Abstract: In this paper, we propose new features for Named Entity Recognition (NER) based on latent semantics. Furthermore, we explore the effect of unsupervised morphological information on these methods and on the NER system in general. The newly created NER system is fully language-independent thanks to the unsupervised nature of the proposed features. We evaluate the system on English, Spanish, Dutch and Czech corpora and study the difference between weakly and highly inflectional languages. Our system achieves the same or even better results than state-of-the-art language dependent systems. The proposed features proved to be very useful and are the main reason of our promising results. (C) 2014 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000350182600015

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Konkol, Michal	B-9206-2016	0000-0002-4041-7148
Brychcin, Tomas	C-1181-2016	0000-0002-7442-0978

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Record 453 of 491

Title: Exploring task-related variability in fMRI data using fluctuations in power spectrum of simultaneously acquired EEG

Author(s): Labounek, R (Labounek, Rene); Lamos, M (Lamos, Martin); Marecek, R (Marecek, Radek); Brazdil, M (Brazdil, Milan); Jan, J (Jan, Jiri)

Source: JOURNAL OF NEUROSCIENCE METHODS **Volume:** 245 **Pages:** 125-136 **DOI:** 10.1016/j.jneumeth.2015.02.016 **Published:** APR 30 2015

Abstract: Background: The paper deals with joint analysis of fMRI and scalp EEG data, simultaneously acquired during event-related oddball experiment. The analysis is based on deriving temporal sequences of EEG powers in individual frequency bands for the selected EEG electrodes and using them as regressors in the general linear model (GLM).
New method: Given the infrequent use of EEG spectral changes to explore task-related variability, we focused on the aspects of parameter setting during EEG regressor calculation and searched for such parameters that can detect task-related variability in EEG-fMRI data. We proposed a novel method that uses relative EEG power in GLM.
Results: Parameter, the type of power value, has a direct impact as to whether task-related variability is detected or not. For relative power, the final results are sensitive to the choice of frequency band of interest. The electrode selection also has certain impact; however, the impact is not crucial. It is insensitive to the choice of EEG power series temporal weighting step. Relative EEG power characterizes the experimental task activity better than the absolute power. Absolute EEG power contains broad spectrum component. Task-related relative power spectral formulas were derived.
Comparison with existing methods: For particular set of parameters, our results are consistent with previously published papers. Our work expands current knowledge by new findings in spectral patterns of different brain processes related to the experimental task.
Conclusions: To make analysis to be sensitive to task-related variability, the parameters type of power value and frequency band should be set properly. (C) 2015 Elsevier B.V. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Brazdil, Milan	D-6836-2012	
Labounek, Rene		0000-0003-0439-1304

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Record 454 of 491

Title: Arabidopsis proteome responses to the smoke-derived growth regulator karrikin

Author(s): Baldrianova, J (Baldrianova, Jana); Cerny, M (Cerny, Martin); Novak, J (Novak, Jan); Jedelsky, PL (Jedelsky, Petr L.); Diviskova, E (Diviskova, Eva); Brzobohaty, B (Brzobohaty, Bretislav)

Source: JOURNAL OF PROTEOMICS **Volume:** 120 **Pages:** 7-20 **DOI:** 10.1016/j.jprot.2015.02.011 **Published:** APR 29 2015

Abstract: Kamkins are butenolide plant growth regulators in smoke from burning plant material that have proven ability to promote germination and seedling photomorphogenesis. However, the molecular mechanisms underlying these processes are unclear. Here we provide the first proteome-wide analysis of early responses to karrikin in plants (Arabidopsis seedlings). Image analysis of two-dimensionally separated proteins, Rubisco-depleted proteomes and phosphoproteomes, together with LC-MS profiling, detected >1900 proteins, 113 of which responded to karrikin treatment. All the differentially abundant proteins (except HSP70-3) are novel karrikin-responders, and most are involved in photosynthesis, carbohydrate metabolism, redox homeostasis, transcription control, proteosynthesis, protein transport and processing, or protein degradation. Our data provide functionally complementary information to previous identifications of karrikin-responsive genes and evidence for a novel karrikin signalling pathway originating in chloroplasts. We present an updated model of karrikin signalling that integrates proteomic data and is supported by growth response observations.
Biological significance
Karrikin has shown promising potential in agricultural applications, yet this process is poorly understood at the molecular level. To the best of our knowledge, this is the first survey of early global proteomic responses to karrikin in plants (Arabidopsis seedlings). The combination of label-free LC-MS profiling and 2-DE analyses provided highly sensitive snapshots of protein abundance and quantitative information on proteoform-level changes. These results present evidence of proteasome-independent karrikin signalling pathways and provide novel targets for detailed mechanistic studies using, e.g., mutants and transgenic plants. (C) 2015 Elsevier B.V. All rights reserved.

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PubMed ID: 25746380
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cerny, Martin	D-7226-2012	
Novak, Jan	I-3635-2014	
Jedelsky, Petr	C-5879-2009	0000-0003-3813-2343
Cerny, Martin		0000-0002-0651-4219

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Record 455 of 491

Title: Site-Specific Analysis of Protein Hydration Based on Unnatural Amino Acid Fluorescence
Author(s): Amaro, M (Amaro, Mariana); Brezovsky, J (Brezovsky, Jan); Kovacova, S (Kovacova, Silvia); Sykora, J (Sykora, Jan); Bednar, D (Bednar, David); Nemec, V (Nemec, Vaclav); Liskova, V (Liskova, Veronika); Kurumbang, NP (Kurumbang, Nagendra Prasad); Beerens, K (Beerens, Koen); Chaloupkova, R (Chaloupkova, Radka); Paruch, K (Paruch, Kamil); Hof, M (Hof, Martin); Damborsky, J (Damborsky, Jiri)
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 137 **Issue:** 15 **Pages:** 4988-4992 **DOI:** 10.1021/jacs.5b01681 **Published:** APR 22 2015
Abstract: Hydration of proteins profoundly affects their functions. We describe a simple and general method for site-specific analysis of protein hydration based on the in vivo incorporation of fluorescent unnatural amino acids and their analysis by steady-state fluorescence spectroscopy. Using this method, we investigate the hydration of functionally important regions of dehalogenases. The experimental results are compared to findings from molecular dynamics simulations.
Accession Number: WOS:000353606700029
PubMed ID: 25815779
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Brezovsky, Jan	C-8290-2012	0000-0001-9677-5078
Hof, Martin	F-5134-2014	0000-0003-2884-3037
Amaro, Mariana	A-4902-2009	0000-0002-4868-227X
Chaloupkova, Radka	M-5565-2016	
Paruch, Kamil	K-7528-2016	
Sykora, Jan	F-5179-2014	
Damborsky, Jiri	H-3799-2012	0000-0002-7848-8216
Beerens, Koen		0000-0001-6608-0443

ISSN: 0002-7863

Record 456 of 491

Title: Intensity dependence of non-linear kinetic behaviour of stimulated Raman scattering in fusion relevant plasmas
Author(s): Masek, M (Masek, Martin); Rohlena, K (Rohlena, Karel)
Source: EUROPEAN PHYSICAL JOURNAL D **Volume:** 69 **Issue:** 4 **Article Number:** 109 **DOI:** 10.1140/epjd/e2015-50853-9 **Published:** APR 16 2015
Abstract: Influence of kinetic effects on 3-wave interaction was examined within the frame of stimulated Raman backward scattering (SRBS) in a rarefied laser corona. The plasma is supposed to be weakly collisional with a negligible density gradient. The model is centred on the physical situation of shock ignition at a large scale direct drive compression experiments. The modelling uses a 1D geometry in a Maxwell-Vlasov model. The method used is a truncated Fourier-Hermite expansion numerically stabilized by a model collisional term with a realistic value of the collision frequency. In parallel, besides the linear theory of SRBS, a coupled mode 3-wave equation system (laser driving wave, Raman back-scattered wave and the daughter forward scattered plasma wave) is solved to demonstrate the correspondence between the full kinetic model and 3-wave interaction with no electron kinetics involved to identify the differences between both the solutions arising due to the electron kinetic effects. We concentrated mainly on the Raman reflectivity, which is one of the important parameters controlling the efficiency of the shock ignition scheme. It was found that the onset of the kinetic effects has a distinct intensity threshold, above which the Raman reflectivity may go down due to the electron kinetics. In addition, we were trying to identify the most important features of the electron phase space behaviour, such as particle trapping in potential minima of the generated plasma wave and its consequences for the 3-wave interaction. The role of the trapped electrons seems to be crucial for a deformation of the plasma wave dispersion curve, as indicated in some earlier work.
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eISSN: 1434-6079

Record 457 of 491

Title: Genetic algorithms for credit scoring: Alternative fitness function performance comparison
Author(s): Kozeny, V (Kozeny, Vaclav)
Source: EXPERT SYSTEMS WITH APPLICATIONS **Volume:** 42 **Issue:** 6 **Pages:** 2998-3004 **DOI:** 10.1016/j.eswa.2014.11.028 **Published:** APR 15 2015
Abstract: Credit scoring methods have been widely investigated by researchers; recently, genetic algorithms have attracted particular attention. Many research papers comparing the performance of genetic algorithms and traditional scoring techniques have been published, but most do not provide enough detail about the fitness function used by the genetic algorithm despite the fact that fitness function has a key influence on the model's overall performance. The aim of this paper is to evaluate the predictive performance of different fitness functions used by genetic algorithms in credit scoring. An alternative fitness function based on a variable bitmask is proposed, and its performance then compared with fitness functions based on a polynomial equation as well as an estimation of parameter range. The results suggest that the bitmask is superior to the two other methods in both accuracy and sensitivity. The Wilcoxon matched-pairs sign rank test and paired t-Test indicate these results are statistically significant.
Accession Number: WOS:000349271500013
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Record 458 of 491

Title: High-throughput physical map anchoring via BAC-pool sequencing
Author(s): Cvikova, K (Cvikova, Katerina); Cattonaro, F (Cattonaro, Federica); Alaux, M (Alaux, Michael); Stein, N (Stein, Nils); Mayer, KFX (Mayer, Klaus F. X.); Dolezel, J (Dolezel, Jaroslav); Bartos, J (Bartos, Jan)
Source: BMC PLANT BIOLOGY **Volume:** 15 **Article Number:** 99 **DOI:** 10.1186/s12870-015-0429-1 **Published:** APR 11 2015
Abstract: Background: Physical maps created from large insert DNA libraries, typically cloned in BAC vector, are valuable resources for map-based cloning and de novo genome sequencing. The maps are most useful if contigs of overlapping DNA clones are anchored to chromosome(s), and ordered along them using molecular markers. Here we present a novel approach for anchoring physical maps, based on sequencing three-dimensional pools of BAC clones from minimum tilling path.
Results: We used physical map of wheat chromosome arm 3DS to validate the method with two different DNA sequence datasets. The first comprised 567 genes ordered along the chromosome arm based on syntenic relationship of wheat with the sequenced genomes of Brachypodium, rice and sorghum. The second dataset consisted of 7,136 SNP-containing sequences, which were mapped genetically in Aegilops tauschii, the donor of the wheat D genome. Mapping of sequence reads from individual BAC pools to the first and the second datasets enabled unambiguous anchoring 447 and 311 3DS-specific sequences, respectively, or 758 in total.
Conclusions: We demonstrate the utility of the novel approach for BAC contig anchoring based on mass parallel sequencing of three-dimensional pools prepared from minimum tilling path of physical map. The existing genetic markers as well as any other DNA sequence could be mapped to BAC clones in a single in silico experiment. The approach reduces significantly the cost and time needed for anchoring and is applicable to any genomic project involving the construction of anchored physical map.
Accession Number: WOS:000353317600001
PubMed ID: 25887276
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bartos, Jan	F-6071-2014	
Mayer, Klaus	M-7941-2015	0000-0001-6484-1077
Dolezel, Jaroslav	B-7716-2008	0000-0002-6263-0492
Stein, Nils	F-7507-2017	0000-0003-3011-8731
Alaux, Michael		0000-0001-9356-4072

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Record 459 of 491

Title: Stepwise Catalytic Mechanism via Short-Lived Intermediate Inferred from Combined QM/MM MERP and PES Calculations on Retaining Glycosyltransferase ppGalNAcT2

Author(s): Trnka, T (Trnka, Tomas); Kozmon, S (Kozmon, Stanislav); Tvaroska, I (Tvaroska, Igor); Koca, J (Koca, Jaroslav)

Source: PLOS COMPUTATIONAL BIOLOGY **Volume:** 11 **Issue:** 4 **Article Number:** e1004061 **DOI:** 10.1371/journal.pcbi.1004061 **Published:** APR 2015

Abstract: The glycosylation of cell surface proteins plays a crucial role in a multitude of biological processes, such as cell adhesion and recognition. To understand the process of protein glycosylation, the reaction mechanisms of the participating enzymes need to be known. However, the reaction mechanism of retaining glycosyltransferases has not yet been sufficiently explained. Here we investigated the catalytic mechanism of human isoform 2 of the retaining glycosyltransferase polypeptide UDP-GalNAc transferase by coupling two different QM/MM-based approaches, namely a potential energy surface scan in two distance difference dimensions and a minimum energy reaction path optimisation using the Nudged Elastic Band method. Potential energy scan studies often suffer from inadequate sampling of reactive processes due to a predefined scan coordinate system. At the same time, path optimisation methods enable the sampling of a virtually unlimited number of dimensions, but their results cannot be unambiguously interpreted without knowledge of the potential energy surface. By combining these methods, we have been able to eliminate the most significant sources of potential errors inherent to each of these approaches. The structural model is based on the crystal structure of human isoform 2. In the QM/MM method, the QM region consists of 275 atoms, the remaining 5776 atoms were in the MM region. We found that ppGalNAcT2 catalyzes a same-face nucleophilic substitution with internal return (SNi). The optimized transition state for the reaction is 13.8 kcal/mol higher in energy than the reactant while the energy of the product complex is 6.7 kcal/mol lower. During the process of nucleophilic attack, a proton is synchronously transferred to the leaving phosphate. The presence of a short-lived metastable oxocarbenium intermediate is likely, as indicated by the reaction energy profiles obtained using high-level density functionals.

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PubMed ID: 25849117

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Kozmon, Stanislav	D-8525-2012	0000-0002-0946-3453
Trnka, Tomas		0000-0002-9273-3820

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Record 460 of 491

Title: Understanding the Electronic Factors Responsible for Ligand Spin-Orbit NMR Shielding in Transition-Metal Complexes

Author(s): Vicha, J (Vicha, Jan); Foroutan-Nejad, C (Foroutan-Nejad, Cina); Pawlak, T (Pawlak, Tomasz); Munzarova, ML (Munzarova, Marketa L.); Straka, M (Straka, Michal); Marek, R (Marek, Radek)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 11 **Issue:** 4 **Pages:** 1509-1517 **DOI:** 10.1021/ct501089z **Published:** APR 2015

Abstract: The significant role of relativistic effects in altering the NMR chemical shifts of light nuclei in heavy-element compounds has been recognized for a long time; however, full understanding of this phenomenon in relation to the electronic structure has not been achieved. In this study, the recently observed qualitative differences between the platinum and gold compounds in the magnitude and the sign of spin-orbit-induced (SO) nuclear magnetic shielding at the vicinal light atom (C-13, N-15), sigma SO(LA), are explained by the contractions of 6s and 6p atomic orbitals in Au complexes, originating in the larger Au nuclear charge and stronger scalar relativistic effects in gold complexes. This leads to the chemical activation of metal 6s and 6p atomic orbitals in Au complexes and their larger participation in bonding with the ligand, which modulates the propagation of metal-induced SO effects on the NMR signal of the LA via the Spin-Orbit/Fermi Contact (SO/FC) mechanism. The magnitude of the sSO(LA) in these square-planar complexes can be understood on the basis of a balance between various metal-based 5d -> 5d* and 6p -> 6p* orbital magnetic couplings. The large and positive sSO(LA) in platinum complexes is dominated by the shielding platinum-based 5d -> 5d* magnetic couplings, whereas small or negative sigma(SO)(LA) in gold complexes is related to the deshielding contribution of the gold-based 6p -> 6p* magnetic couplings. Further, it is demonstrated that sigma(SO)(LA) correlates quantitatively with the extent of M-LA electron sharing that is the covalence of the M-LA bond (characterized by the QTAIM delocalization index, DI). The present findings will contribute to further understanding of the origin and propagation of the relativistic effects influencing the experimental NMR parameters in heavy-element systems.

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PubMed ID: 26574362

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Straka, Michal	E-5246-2011	0000-0002-7857-4990
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Vicha, Jan	D-8417-2012	0000-0003-3698-8236

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Record 461 of 491

Title: PHYLOGENETIC ANALYSIS OF CULTIVATION-RESISTANT TERRESTRIAL CYANOBACTERIA WITH MASSIVE SHEATHS (STIGONEMA SPP. AND PETALONEMA ALATUM, NOSTOCALES, CYANOBACTERIA) USING SINGLE-CELL AND FILAMENT SEQUENCING OF ENVIRONMENTAL SAMPLES

Author(s): Mares, J (Mares, Jan); Lara, Y (Lara, Yannick); Dadakova, I (Dadakova, Iva); Hauer, T (Hauer, Tomas); Uher, B (Uher, Bohuslav); Wilmotte, A (Wilmotte, Annick); Kastovsky, J (Kastovsky, Jan)

Source: JOURNAL OF PHYCOLOGY **Volume:** 51 **Issue:** 2 **Pages:** 288-297 **DOI:** 10.1111/jpy.12273 **Published:** APR 2015

Abstract: Molecular assessment of a large portion of traditional cyanobacterial taxa has been hindered by the failure to isolate and grow them in culture. In this study, we developed an optimized protocol for single cell/filament isolation and 16S rRNA gene sequencing of terrestrial cyanobacteria with large mucilaginous sheaths, and applied it to determine the phylogenetic position of typical members of the genera Petalonema and Stigonema. A methodology based on a glass-capillary isolation technique and a semi-nested PCR protocol enabled reliable sequencing of the 16S rRNA gene from all samples analyzed. Ten samples covering seven species of Stigonema from Europe, North and Central America, and Hawaii, and the type species of Petalonema from Slovakia were sequenced. Contrary to some previous studies, which proposed a relationship with heteropolar nostocalean cyanobacteria, Petalonema appeared to belong to the family Scytonemataceae. Analysis of Stigonema specimens recovered a unique coherent phylogenetic cluster, substantially broadening our knowledge of the molecular diversity within this genus. Neither the uni- to biseriate species nor the multiseriate species formed monophyletic subclusters within the genus. Typical multiseriate species of Stigonema clustered in a phylogenetic branch derived from uni- to biseriate S. ocellatum Thuret ex Bornet & Flahault in our analysis, suggesting that species with more complex thalli may have evolved from the more simple ones. We propose the technique tested in this study as a promising tool for a future revision of the molecular taxonomy in cyanobacteria.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Hauer, Tomas	F-5089-2010	0000-0002-8005-5874
Mares, Jan	B-2395-2009	0000-0002-5745-7023

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Record 462 of 491

Title: Application of ab-initio molecular electronic structure calculations of radiolytic and hydrolytic stabilities of prospective extractants

Author(s): Koubsky, T (Koubsky, Tomas); Kalvoda, L (Kalvoda, Ladislav)

Source: JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY **Volume:** 304 **Issue:** 1 **Pages:** 227-235 **DOI:** 10.1007/s10967-014-3600-5 **Published:** APR 2015

Abstract: For theoretical estimation of the general and local chemical stability of m-xylylene-bis-diglycolamide and its degradation products the ab-initio calculations were performed, using the Gaussian and DMol(3) codes. The chemical stability was assessed according to the stability indicators, such as HOMO-LUMO gap, spatial localization of HOMO, electrostatic potential, atomic charges, and bond orders. The results of various methods are in good agreement with the published experimental stability studies. Such theoretical predictions can provide a valuable support to experimental scientists in development of novel extraction methods and stable extractants of actinide and lanthanide ions.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kalvoda, Ladislav		0000-0002-4051-7093

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Record 463 of 491

Title: Computational study of missense mutations in phenylalanine hydroxylase

Author(s): Reblova, K (Reblova, Kamila); Kulhanek, P (Kulhanek, Petr); Fajkusova, L (Fajkusova, Lenka)

Source: JOURNAL OF MOLECULAR MODELING **Volume:** 21 **Issue:** 4 **Article Number:** 70 **DOI:** 10.1007/s00894-015-2620-6 **Published:** APR 2015

Abstract: Hyperphenylalaninemia (HPA) is one of the most common metabolic disorders. HPA, which is transmitted by an autosomal recessive mode of inheritance, is caused by mutations of the phenylalanine hydroxylase gene. Most mutations are missense and lead to reduced protein stability and/or impaired catalytic function. The impact of such mutations varies, ranging from classical phenylketonuria (PKU), mild PKU, to non-PKU HPA phenotypes. Despite the fact that HPA is a monogenic disease, clinical data show that one PKU genotype can be associated with more in vivo phenotypes, which indicates the role of other (still unknown) factors. To better understand the phenotype-genotype relationships, we analyzed computationally the impact of missense mutations in homozygotes stored in the BIOPKU database. A total of 34 selected homozygous genotypes was divided into two main groups according to their phenotypes: (A) genotypes leading to non-PKU HPA or combined phenotype non-PKU HPA/mild PKU and (B) genotypes leading to classical PKU, mild PKU or combined phenotype mild PKU/classical PKU. Combining in silico analysis and molecular dynamics simulations (in total 3 mu s) we described the structural impact of the mutations, which allowed us to separate 32 out of 34 mutations between groups A and B. Testing the simulation conditions revealed that the outcome of mutant simulations can be modulated by the ionic strength. We also employed programs SNPs3D, Polyphen-2, and SIFT but based on the predictions performed we were not able to discriminate mutations with mild and severe PKU phenotypes.

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PubMed ID: 25750018

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kulhanek, Petr	D-6884-2012	0000-0002-4152-6514

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Record 464 of 491

Title: Electrolyte pore/solution partitioning by expanded grand canonical ensemble Monte Carlo simulation

Author(s): Moucka, F (Moucka, Filip); Bratko, D (Bratko, Dusan); Luzar, A (Luzar, Alenka)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 142 **Issue:** 12 **Article Number:** 124705 **DOI:** 10.1063/1.4914461 **Published:** MAR 28 2015

Abstract: Using a newly developed grand canonical Monte Carlo approach based on fractional exchanges of dissolved ions and water molecules, we studied equilibrium partitioning of both components between laterally extended apolar confinements and surrounding electrolyte solution. Accurate calculations of the Hamiltonian and tensorial pressure components at anisotropic conditions in the pore required the development of a novel algorithm for a self-consistent correction of nonelectrostatic cut-off effects. At pore widths above the kinetic threshold to capillary evaporation, the molality of the salt inside the confinement grows in parallel with that of the bulk phase, but presents a nonuniform width-dependence, being depleted at some and elevated at other separations. The presence of the salt enhances the layered structure in the slit and lengthens the range of inter-wall pressure exerted by the metastable liquid. Solvation pressure becomes increasingly repulsive with growing salt molality in the surrounding bath. Depending on the sign of the excess molality in the pore, the wetting free energy of pore walls is either increased or decreased by the presence of the salt. Because of simultaneous rise in the solution surface tension, which increases the free-energy cost of vapor nucleation, the rise in the apparent hydrophobicity of the walls has not been shown to enhance the volatility of the metastable liquid in the pores. (C) 2015 AIP Publishing LLC.

Accession Number: WOS:000352316700045
PubMed ID: 25833601

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Bratko, Dusan	F-5687-2010	0000-0002-3675-5275
Moucka, Filip	M-4013-2013	0000-0002-1400-7890

ISSN: 0021-9606
eISSN: 1089-7690

Record 465 of 491

Title: Exploring Reaction Pathways for O-GlcNAc Transferase Catalysis. A String Method Study

Author(s): Kumari, M (Kumari, Manju); Kozmon, S (Kozmon, Stanislav); Kulhanek, P (Kulhanek, Petr); Stepan, J (Stepan, Jakub); Tvaroska, I (Tvaroska, Igor); Koca, J (Koca, Jaroslav)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 119 **Issue:** 12 **Pages:** 4371-4381 **DOI:** 10.1021/jp511235f **Published:** MAR 26 2015

Abstract: The inverting O-GlcNAc glycosyltransferase (OGT) is an important post-translation enzyme, which catalyzes the transfer of N-acetylglucosamine from UDP-N-acetylglucosamine (UDP-GlcNAc) to the hydroxyl group of the Ser/Thr of cytoplasmic, nuclear, and mitochondrial proteins. In the past, three different catalytic bases were proposed for the reaction: His498, alpha-phosphate, and Asp554. In this study, we used hybrid quantum mechanics/molecular mechanics (QM/MM) Car-Parrinello molecular dynamics to investigate reaction paths using alpha-phosphate and Asp554 as the catalytic bases. The string method was used to calculate the free-energy reaction profiles of the tested mechanisms. During the investigations, an additional mechanism was observed. In this mechanism, a proton is transferred to alpha-phosphate via a water molecule. Our calculations show that the mechanism with alpha-phosphate acting as the base is favorable. This reaction has a rate-limiting free-energy barrier of 23.5 kcal/mol, whereas reactions utilizing Asp554 and water-assisted alpha-phosphate have barriers of 41.7 and 40.9 kcal/mol, respectively. Our simulations provide a new insight into the catalysis of OGT and may thus guide rational drug design of transition-state analogue inhibitors with potential therapeutic use.

Accession Number: WOS:000351971100004
PubMed ID: 25731954

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Kulhanek, Petr	D-6884-2012	0000-0002-4152-6514
Kozmon, Stanislav	D-8525-2012	0000-0002-0946-3453

ISSN: 1520-6106

Record 466 of 491

Title: Host specificity of turkey and chicken Eimeria: Controlled cross-transmission studies and a phylogenetic view

Author(s): Vrba, V (Vrba, Vladimir); Pakandl, M (Pakandl, Michal)

Source: VETERINARY PARASITOLOGY **Volume:** 208 **Issue:** 3-4 **Pages:** 118-124 **DOI:** 10.1016/j.vetpar.2015.01.017 **Published:** MAR 15 2015

Abstract: Protozoan parasites of the Eimeria genus have undergone extensive speciation and are now represented by a myriad of species that are specialised to different hosts. These species are highly host-specific and usually parasitise single host species, with only few reported exceptions. Doubts regarding the strict host specificity were frequent in the original literature describing coccidia parasitising domestic turkeys. The availability of pure characterised lines of turkey and chicken Eimeria species along with the recently developed quantitative PCR identification of these species allowed to investigate the issue of host specificity using well-controlled cross-transmission experiments. Seven species of gallinaceous birds (Gallus gallus, Meleagris gallopavo, Alectoris rufa, Perdix perdix, Phasianus colchicus, Numida meleagris and Colinus virginianus) were inoculated with six species and strains of turkey Eimeria and six species of chicken coccidia and production of oocysts was monitored. Turkey Eimeria species E. dispersa, E. innocua and E. meleagridis could complete their development in the hosts from different genera or even different families. Comparison of phylogenetic positions of these Eimeria species according to 18S rDNA and COI showed that the phylogeny cannot explain the observed patterns of host specificity. These findings suggest that the adaptation of Eimeria parasites to foreign hosts is possible and might play a significant role in the evolution and diversification of this genus. (C) 2015 Elsevier B.V. All rights reserved.

Accession Number: WOS:000351644400002

PubMed ID: 25660426

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Vrba, Vladimir		0000-0002-2682-2809

ISSN: 0304-4017

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Record 467 of 491

Title: Coarse-Grain Simulations of Skin Ceramide NS with Newly Derived Parameters Clarify Structure of Melted Phase

Author(s): Sovova, Z (Sovova, Zofie); Berka, K (Berka, Karel); Otyepka, M (Otyepka, Michal); Jurecka, P (Jurecka, Petr)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 119 **Issue:** 10 **Pages:** 3988-3998 **DOI:** 10.1021/jp5092366 **Published:** MAR 12 2015

Abstract: Ceramides are lipids that are involved in numerous biologically, important structures (e.g., the strafuni comeum and ceramide-rich platforms) and processes (e.g., signal ttankluction and, membrane fusion), but their behavior is not fully understood. We report coarse-grain force, field parameters for N-lignoteryl-sphingosine (cerainide NS, also known as cerainide 2) that are consistent with the Martini force field. These parameterSimere optimized for simulation in the gel phase and validated against atbmistic srpiulations Coarse-grained simulations with our parameters provide areas per lipid, membrane thicknesses, and electron density profiles that are in good agreement with atomistic simulations. Properties of the ulated membranes are compared with available,experiniental,data. The obtained parameters were used to model the phase behavior of,Ceraiiiide NS as a funetion of ternperature and hydration. At low Water content and above the main phase transition temperature, the bilayet, melts into an irregular phase, which May correspond to the Unstructured melted-chain phase observed in X-ray diffraction experiments. The developed parameters, also reproduce the extended,conformation of ceramide, which may occur in the stratum comeum. The parameters presented herein will-facllitate studies on important complex functional structure such as the uppermost layer of the skin and ceramide-rich platforms in phospholipid membranes.

Accession Number: WOS:000351188300012

PubMed ID: 25679231

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Otyepka, Michal	D-1220-2017	0000-0002-1066-5677
Berka, Karel	E-2839-2010	0000-0001-9472-2589
Otyepka, Michal	A-5922-2008	

ISSN: 1520-6106

Record 468 of 491

Title: Comment on "Some Unexpected Behavior of the Adsorption of Alkali Metal Ions onto the Graphene Surface under the Effect of External Electric Field"

Author(s): Foroutan-Nejad, C (Foroutan-Nejad, Cina); Novak, M (Novak, Martin); Marek, R (Marek, Radek)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 119 **Issue:** 10 **Pages:** 5752-5754 **DOI:** 10.1021/jp511541p **Published:** MAR 12 2015

Accession Number: WOS:000351189100059

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Novak, Martin	I-3248-2015	0000-0001-5067-1994
Marek, Radek	D-6929-2012	0000-0002-3668-3523

ISSN: 1932-7447

Record 469 of 491

Title: Fully automated pipeline for detection of sex linked genes using RNA-Seq data

Author(s): Michalovova, M (Michalovova, Monika); Kubat, Z (Kubat, Zdenek); Hobza, R (Hobza, Roman); Vyskot, B (Vyskot, Boris); Kejnovsky, E (Kejnovsky, Eduard)

Source: BMC BIOINFORMATICS **Volume:** 16 **Article Number:** 78 **DOI:** 10.1186/s12859-015-0509-0 **Published:** MAR 11 2015

Abstract: Background: Sex chromosomes present a genomic region which to some extent, differs between the genders of a single species. Reliable high-throughput methods for detection of sex chromosomes specific markers are needed, especially in species where genome information is limited. Next generation sequencing (NGS) opens the door for identification of unique sequences or searching for nucleotide polymorphisms between datasets. A combination of classical genetic segregation analysis along with RNA-Seq data can present an ideal tool to map and identify sex chromosome-specific expressed markers. To address this challenge, we established genetic cross of dioecious plant Rumex acetosa and generated RNA-Seq data from both parental generation and male and female offspring.

Results: We present a pipeline for detection of sex linked genes based on nucleotide polymorphism analysis. In our approach, tracking of nucleotide polymorphisms is carried out using a cross of preferably distant populations. For this reason, only 4 datasets are needed - reads from high-throughput sequencing platforms for parent generation (mother and father) and F1 generation (male and female progeny). Our pipeline uses custom scripts together with external assembly, mapping and variant calling software. Given the resource-intensive nature of the computation, servers with high capacity are a requirement. Therefore, in order to keep this pipeline easily accessible and reproducible, we implemented it in Galaxy - an open, web-based platform for data-intensive biomedical research. Our tools are present in the Galaxy Tool Shed, from which they can be installed to any local Galaxy instance. As an output of the pipeline, user gets a FASTA file with candidate transcriptionally active sex-linked genes, sorted by their relevance. At the same time, a BAM file with identified genes and alignment of reads is also provided. Thus, polymorphisms following segregation pattern can be easily visualized, which significantly enhances primer design and subsequent steps of wet-lab verification.

Conclusions: Our pipeline presents a simple and freely accessible software tool for identification of sex chromosome linked genes in species without an existing reference genome. Based on combination of genetic crosses and RNA-Seq data, we have designed a high-throughput, cost-effective approach for a broad community of scientists focused on sex chromosome structure and evolution.

Accession Number: WOS:000351341600001

PubMed ID: 25884927

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Hobza, Roman	I-4297-2014	
Kubat, Zdenek	D-9221-2012	0000-0001-8278-9495

ISSN: 1471-2105

Record 470 of 491

Title: Electron-Deficient Heteroarenium Salts: An Organocatalytic Tool for Activation of Hydrogen Peroxide in Oxidations

Author(s): Sturala, J (Sturala, Jiri); Bohacova, S (Bohacova, Sona); Chudoba, J (Chudoba, Josef); Metelkova, R (Metelkova, Radka); Cibulka, R (Cibulka, Radek)

Source: JOURNAL OF ORGANIC CHEMISTRY **Volume:** 80 **Issue:** 5 **Pages:** 2676-2699 **DOI:** 10.1021/jo502865f **Published:** MAR 6 2015

Abstract: A series of monosubstituted pyrimidinium and pyrazinium triflates and 3,5-disubstituted pyridinium triflates were prepared and tested as simple catalysts of oxidations with hydrogen peroxide, using sulfoxidation as a model reaction. Their catalytic efficiency strongly depends on the type of substituent and is remarkable for derivatives with an electron-withdrawing group, showing reactivity comparable to that of flavinium salts which are the prominent organocatalysts for oxygenations. Because of their high stability and good accessibility, 4-(trifluoromethyl)pyrimidinium and 3,5-dinitropyridinium triflates are the catalysts of choice and were shown to catalyze oxidation of aliphatic and aromatic sulfides to sulfoxides, giving quantitative conversions, high preparative yields and excellent chemoselectivity. The high efficiency of electron-poor heteroarenium salts is rationalized by their ability to readily form adducts with nucleophiles, as documented by low pK(R+) values (pK(R+) < 5) and less negative reduction potentials (E-red > -0.5 V). Hydrogen peroxide adducts formed in situ during catalytic oxidation act as substrate oxidizing agents. The Gibbs free energies of oxygen transfer from these heterocyclic hydroperoxides to thioanisole, obtained by calculations at the B3LYP/6-311++g(d,p) level, showed that they are much stronger oxidizing agents than alkyl hydroperoxides and in some cases are almost comparable to derivatives of flavin hydroperoxide acting as oxidizing agents in monooxygenases.

Accession Number: WOS:000350841600022

PubMed ID: 25658679

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Cibulka, Radek	H-1298-2016	0000-0002-8584-7715
Sturala, Jiri	G-8229-2017	0000-0002-8113-0709
Sturala, Jiri	A-1253-2013	

ISSN: 0022-3263

Record 471 of 491

Title: Electronic structure, chemical bonding and optical properties of Di-2-pyrymidonium dichloride diiodide (C4H5ClIN2O) from first-principles

Author(s): Azam, S (Azam, Sikander); Reshak, AH (Reshak, A. H.)

Source: MATERIALS SCIENCE IN SEMICONDUCTOR PROCESSING **Volume:** 31 **Pages:** 372-379 **DOI:** 10.1016/j.mssp.2014.12.009 **Published:** MAR 2015

Abstract: The electronic structure and electronic charge density of the monoclinic phase Di-2-pyrymidonium dichloride-di-iodide compound is studied by using the local density approximation (LDA) and Engel Vosko generalized gradient approximation (EVGGA). Using LDA for exchange correlation potential, we have optimized the atomic positions taken from the X-ray crystallographic data by minimization of the forces acting on the atoms. From the relaxed geometry the electronic structure, electronic charge density and the optical properties were determined. Band structures disclose that this compound has indirect energy band gap. The obtained energy band gap value using EVGGA (2.010 eV) is larger than that obtained within LDA (1.781 eV). To envision the chemical bonding nature between the composition of the investigated compound, the distribution of charge density was discussed in the (-1 0 1) crystallographic plane. The contour plot shows partial ionic and strong covalent bonding between C-O, N-C and C-H atoms. The optical properties of Di-2-pyrymidonium dichloride-di-iodide are obtained by the calculation of the dielectric function. (C) 2014 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000350513500052

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363
Azam, Sikander		0000-0001-5923-1127

ISSN: 1369-8001

eISSN: 1873-4081

Record 472 of 491

Title: Roholtiella, gen. nov (Nostocales, Cyanobacteria)-a tapering and branching cyanobacteria of the family Nostocaceae

Author(s): Bohunicka, M (Bohunicka, Marketa); Pietrasiak, N (Pietrasiak, Nicole); Johansen, JR (Johansen, Jeffrey R.); Gomez, EB (Gomez, Esther Berrendero); Hauer, T (Hauer, Tomas); Gaysina, LA (Gaysina, Lira A.); Lukesova, A (Lukesova, Alena)

Source: PHYTOTAXA **Volume:** 197 **Issue:** 2 **Pages:** 84-103 **DOI:** 10.11646/phytotaxa.197.2.2 **Published:** FEB 11 2015

Abstract: A total of 16 strains phylogenetically placed within the Nostocaceae were found to possess morphological features of the Rivulariaceae and Tolypothrichaceae (tapering trichomes and single false branching, respectively) in addition to their typical Nostocacean features (production of arthrospores in series). These strains formed a strongly supported clade separate from other strains that are phylogenetically and morphologically close. We describe four new species within the genus Roholtiella gen. nov. The four species include three distinguishable morphotypes. Roholtiella mojaviensis and R. edaphica are morphologically distinct from each other and from the other two species, R. fluviatilis and R. bashkiriorum. Roholtiella fluviatilis and R. bashkiriorum are cryptic species with respect to each other. All four species are easily distinguished based on the sequence of the 16S-23S ITS regions, in particular the flanking regions to the conserved Box-B and V3 helices. The species are further established by the elevated p-distance between species that is much reduced among strains within the same species. Calochaete cimrmanii, a recently described tapering species from tropical biomes, is the most likely sister taxon to Roholtiella.

Accession Number: WOS:000350225100002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Lukesova, Alena	G-1451-2014	
Hauer, Tomas	F-5089-2010	0000-0002-8005-5874
Johansen, Jeffrey	F-5616-2011	0000-0002-0794-9417
Gaysina, Lira		0000-0002-0920-6449

ISSN: 1179-3155

eISSN: 1179-3163

Record 473 of 491

Title: Hyperfine Fields and Lattice Deformations in Ba and Sr Hexaferrites

Author(s): Chlan, V (Chlan, V.); Kouril, K (Kouril, K.); Stepankova, H (Stepankova, H.)

Source: ACTA PHYSICA POLONICA A **Volume:** 127 **Issue:** 2 **Pages:** 594-596 **DOI:** 10.12693/APhysPolA.127.594 **Published:** FEB 2015

Abstract: Hyperfine magnetic fields on Fe-57 nuclei in Sr and Ba hexagonal ferrites are calculated in dependence on unit cell volume and c/a ratio. By analysing the local deformations of Fe-O-Fe triads the results are explained as changes to contact hyperfine field due to Fe-O covalency effects and supertransferred hyperfine fields. Most pronounced effect is found for bipyramidal iron Fe(b) where the total contact field is reduced due to noticeable shortening of Fe(b)-O bonds.

Accession Number: WOS:000352139600144

Conference Title: 14th European Conference on Physics of Magnetism (PM)

Conference Date: JUN 23-27, 2014

Conference Location: Poznan, POLAND

Conference Sponsors: Polish Acad Sci, Inst Mol Phys, Adam Mickiewicz Univ, Fac Phys

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Stepankova, Helena	P-2352-2017	0000-0002-4051-2495
Chlan, Vojtech	D-4868-2017	0000-0001-6963-9273

ISSN: 0587-4246

eISSN: 1898-794X

Record 474 of 491

Title: Shell galaxies as laboratories for testing MOND

Author(s): Bilek, M (Bilek, M.); Ebrova, I (Ebrova, I.); Jungwiert, B (Jungwiert, B.); Jilkova, L (Jilkova, L.); Bartoskova, K (Bartoskova, K.)

Source: CANADIAN JOURNAL OF PHYSICS **Volume:** 93 **Issue:** 2 **Special Issue:** SI **Pages:** 203-212 **DOI:** 10.1139/cjp-2014-0170 **Published:** FEB 2015

Abstract: Tests of MOND in elliptical galaxies are relatively rare because they often lack kinematic tracers in the regions where MOND effects are significant. Stellar shells observed in many elliptical galaxies offer a promising way to constrain their gravitational fields. Shells appear as glowing arcs around the host galaxy, with radii observed up to similar to 100 kpc. The stars in axially symmetric shell systems move in nearly radial orbits. The radial distributions of shell locations and the spectra of stars in shells can be used to constrain the gravitational potential of their host galaxy. The symmetrical shell systems, being especially suitable for these studies, occur in approximately 3% of all early-type galaxies. Hence, if we overcome several problems (e.g., multiple shell generations present in the system, shells missed by observations, blurry shell edges, dynamical friction during the merger), the shells substantially increase the number of ellipticals in which MOND can be tested up to large radii. In this paper, we review our work on shell galaxies in MOND. We summarize Bilek et al. (Astron. Astrophys. 559, A110 (2013)), where we demonstrated the consistency of shell radii in an elliptical NGC 3923 with MOND, and Bilek et al. (arXiv:1404.1109. 2014), in which we predicted a giant (similar to 200 kpc), yet undiscovered shell of NGC 3923. We explain the shell identification method that was used in these two papers. We further describe the expected shape of line profiles in shell spectra in MOND, which is very special because of the direct relation of the gravitational field and baryonic matter distribution (Bilek et al. 2014, in preparation).

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ISSN: 0008-4204

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Record 475 of 491

Title: MDPV: metric distance permutation vocabulary

Author(s): Dohnal, V (Dohnal, Vlastislav); Homola, T (Homola, Tomas); Zezula, P (Zezula, Pavel)

Source: INFORMATION RETRIEVAL **Volume:** 18 **Issue:** 1 **Pages:** 51-72 **DOI:** 10.1007/s10791-014-9247-6 **Published:** FEB 2015

Abstract: Sub-image content-based similarity search forms an important operation in current image archives since it provides users with images that contain a query image as their part. Such a search can conveniently be implemented using the bag-of-features model. Its integral part is a construction of visual vocabulary. Most existing algorithms to create a visual vocabulary suffer from high computational (e.g. k-means) or supervisor-guidance (e.g. visual-bit classifier, or sparse coding) requirements. In this paper, we propose a novel approach to visual vocabulary construction called metric distance permutation vocabulary. It is based on permutations of metric distances to create compact visual words. Its major advantage over prior techniques is time and space efficiency of vocabulary construction and quantization process during querying, while achieving comparable or even better effectiveness (query result quality). Moreover, this basic concept is extended to combine more independent permutations. Both the proposals are experimented on well-known real-world data-sets and compared to other state-of-the-art techniques.

Accession Number: WOS:000348350600003

ISSN: 1386-4564

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Record 476 of 491

Title: Tuning the Spectroscopic Properties of Aryl Carotenoids by Slight Changes in Structure

Author(s): Fuciman, M (Fuciman, Marcel); Kesan, G (Kesan, Guerkan); LaFountain, AM (LaFountain, Amy M.); Frank, HA (Frank, Harry A.); Polivka, T (Polivka, Tomas)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 119 **Issue:** 4 **Pages:** 1457-1467 **DOI:** 10.1021/jp512354r **Published:** JAN 29 2015

Abstract: Two carotenoids with aryl rings were studied by femtosecond transient absorption spectroscopy and theoretical computational methods, and the results were compared with those obtained from their nonaryl counterpart, beta-carotene. Although isorenieratene has more conjugated C-C bonds than beta-carotene, its effective conjugation length, Neff, is shorter than of b-carotene. This is evidenced by a longer S-1 lifetime and higher S-1 energy of isorenieratene compared to the values for beta-carotene. On the other hand, although isorenieratene and renierapurpurin have the same pi-electron conjugated chain structure, Neff is different for these two carotenoids. The S-1 lifetime of renierapurpurin is shorter than that of isorenieratene, indicating a longer Neff for renierapurpurin. This conclusion is also consistent with a lower S-1 energy of renierapurpurin compared to those of the other carotenoids. Density functional theory (DFT) was used to calculate equilibrium geometries of ground and excited states of all studied carotenoids. The terminal ring torsion in the ground state of isorenieratene (41 degrees) is very close to that of beta-carotene (45 degrees), but equilibration of the bond lengths within the aryl rings indicates that the each aryl ring forms its own conjugated system. This results in partial detachment of the aryl rings from the overall conjugation making Neff of isorenieratene shorter than that of beta-carotene. The different position of the methyl group at the aryl ring of renierapurpurin diminishes the aryl ring torsion to similar to 20 degrees. This planarization results in a longer Neff than that of isorenieratene, rationalizing the observed differences in spectroscopic properties.

Accession Number: WOS:000348753600022

PubMed ID: 25558974

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Polivka, Tomas	G-9564-2014	0000-0002-6176-0420
KESAN, Gurkan	G-4760-2012	0000-0002-4173-8250
LaFountain, Amy		0000-0003-0583-2044

ISSN: 1520-6106

Record 477 of 491

Title: Is NICS a reliable aromaticity index for transition metal clusters?

Author(s): Foroutan-Nejad, C (Foroutan-Nejad, Cina)

Source: THEORETICAL CHEMISTRY ACCOUNTS **Volume:** 134 **Issue:** 2 **Article Number:** 8 **DOI:** 10.1007/s00214-015-1617-7 **Published:** JAN 17 2015

Abstract: In the present account the nature of aromaticity/antiaromaticity of fourteen metallic complexes/clusters are reexamined. These species were classified as aromatic by means of different nucleus independent chemical shift (NICS) based approaches, previously. Visualization of the current density and magnetizability of atomic basins reveals that none of the studied systems are magnetic aromatic, i.e. sustain diamagnetic ring current. It is demonstrated that negative NICS values near the ring plane of the studied molecules originates from remarkably strong local paramagnetic current around their transition metal atom nuclei. This phenomenon has been observed only for Sc3-all-metal cluster but current study demonstrates that the influence of the local paramagnetic currents around transition metal atoms on NICS is a general phenomenon that must be carefully considered prior to classification of the metallic systems as aromatic. Furthermore, this study suggests that NICS is not a reliable aromaticity index for transition-metal clusters/molecules.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173

ISSN: 1432-881X

eISSN: 1432-2234

Record 478 of 491

Title: On the solid-state NMR spectra of naproxen

Author(s): Czernek, J (Czernek, Jiri)

Source: CHEMICAL PHYSICS LETTERS **Volume:** 619 **Pages:** 230-235 **DOI:** 10.1016/j.cplett.2014.11.031 **Published:** JAN 5 2015

Abstract: Two previous measurements of the C-13 and H-1 NMR isotropic chemical shifts in crystalline naproxen, which is an important pharmaceutical compound, are confronted with the results obtained from several theoretical approaches capable of the proper treatment of solid-phase effects. In the underlying geometrical optimizations, two crystal structures are considered. The agreement between the data sets is quantified, including an evaluation of the similarity between the experimental solid-state NMR spectra. The C-13-H-1 heteronuclear correlations are analyzed, and their various assignments are discussed employing the statistical treatment of the differences between the measured and theoretical isotropic chemical shifts. (C) 2014 Elsevier B.V. All rights reserved.

Accession Number: WOS:000347104600045

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Czernek, Jiri	H-6708-2014	

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eISSN: 1873-4448

Record 479 of 491

Title: Ferrous and ferric state of cytochromes P450 in intact Escherichia coli cells: a possible role of cytochrome P450-flavodoxin interactions

Author(s): Culka, M (Culka, Martin); Milichovsky, J (Milichovsky, Jan); Jerabek, P (Jerabek, Petr); Stiborova, M (Stiborova, Marie); Martinek, V (Martinek, Vaclav)

Source: NEUROENDOCRINOLOGY LETTERS **Volume:** 36 **Pages:** 29-37 **Supplement:** 1 **Published:** 2015

Abstract: OBJECTIVES: Cytochromes P450 (CYPs) are heme enzymes oxygenating a broad range of substrates. Their activity is dependent on the presence of a suitable electron donor (eukaryotic NADPH: CYP oxidoreductase or cytochrome b5). The Escherichia naturally contain no CYPs and no NADPH: CYP oxidoreductase, however it was reported that some CYPs heterologously expressed in E. coli may exist in the ferrous form. A small bacterial flavoprotein, flavodoxin is considered to be responsible for reduction some of these CYPs.
METHODS: The reduction state of several human CYPs expressed in the intact living E. coli cells was examined. In addition, molecular dynamics and steered molecular dynamics simulations were performed to predict and compare affinity of flavodoxin toward selected CYPs.
RESULTS: We determined the reduction state of five human CYPs heterologously expressed in E. coli. The computationally predicted stabilities of CYP-flavodoxin complexes correlate with the percentage of reduced CYPs in bacterial cells. The mean electron transfer distance within optimized complexes was also related to the percentage of reduced CYPs.
CONCLUSION: Depending on the resting state, the CYPs heterologously expressed in E. coli could be divided into two groups; CYP2C8, 2C9, 3A4 are in E. coli present mainly in the oxidized form; while CYP1A1, 1A2, 2A6, 2A13, 2B6, 2D6 are found predominantly in the reduced form. We found a significant correlation between the stability of CYP-flavodoxin complexes and the percentage of reduced CYPs in bacteria. Hence, the naturally expressed flavodoxin is probably responsible for reduction of a larger group of human CYPs in bacterial cells.

Accession Number: WOS:000369404400004
PubMed ID: 26757119
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Stiborova, Marie	A-5982-2015	0000-0001-5430-4403
Martinek, Vaclav	E-6710-2011	0000-0003-3321-4526
Jerabek, Petr	A-1223-2013	0000-0002-5175-6890

ISSN: 0172-780X

Record 480 of 491

Title: Analytical investigations of CdS nanostructures for optoelectronic applications

Author(s): Al-Douri, Y (Al-Douri, Y.); Reshak, AH (Reshak, A. H.)

Source: OPTIK **Volume:** 126 **Issue:** 24 **Pages:** 5109-5114 **DOI:** 10.1016/j.ijleo.2015.09.233 **Published:** 2015

Abstract: Cadmium sulfide (CdS) nanostructures were prepared and deposited on glass substrates of Cd:S (1.2-0.05 mol/L) annealed at 400 degrees C with different spin coating speed (1000, 3000 and 5000 rpm) using spin coating technique. Structural, morphological and analytical studies were investigated by X-ray diffraction (XRD), atomic force microscopy (AFM), Fourier transform infrared (FTIR) and UV-Vis Spectroscopy. It is found that the particle size of CdS nanostructures is 1.40, 1.78 and 2.31 nm prepared at 1000, 3000 and 5000 rpm, respectively. The band gap was measured with an indication of transmission within the visible range; it is changed due to particle size of CdS nanostructures. The calculated refractive index and optical dielectric constant results give agreement with experimental results. The obtained results are in accordance with experimental and theoretical data. (C) 2015 Elsevier GmbH. All rights reserved.

Accession Number: WOS:000368650800064
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Reshak, Ali	B-8649-2008	0000-0001-9426-8363

ISSN: 0030-4026

Record 481 of 491

Title: Modelling of phase diagrams of nanoalloys with complex metallic phases: application to Ni-Sn

Author(s): Kroupa, A (Kroupa, A.); Kana, T (Kana, T.); Bursik, J (Bursik, J.); Zemanova, A (Zemanova, A.); Sob, M (Sob, M.)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 17 **Issue:** 42 **Pages:** 28200-28210 **DOI:** 10.1039/c5cp00281h **Published:** 2015

Abstract: A method for modelling of size-dependent phase diagrams was developed by combining the semiempirical CALPHAD method and ab initio calculations of surface stresses for intermetallic phases. A novel approach was devised for the calculation of surface energy, free of systematic errors from the selection of different parameters of the software (e.g. number of the k-points) and for handling layered structures and off-stoichiometric slabs. Our approach allows the determination of complex size-dependent phase diagrams of systems with intermetallic phases, which was not possible up to now. The method was verified for the modelling of the phase diagram of the Ni-Sn system and basic comparison with rare experimental results was shown. There is reasonable agreement between the calculated and experimental results. The modelling of size-dependent phase diagrams of real systems allows the prediction of phase equilibria existing in nanosystems and possible changes in material properties. There is a need for such knowledge and the existence of reliable data for simpler systems is crucial for further application of this approach. This should motivate future experimental work.

Accession Number: WOS:000363686800031
PubMed ID: 25824490
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kroupa, Ales	A-1162-2014	
Kana, Tomas	G-1645-2014	
Bursik, Jiri	B-8684-2013	0000-0002-6749-9788

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eISSN: 1463-9084

Record 482 of 491

Title: On the non-classical contribution in lone-pair-pi interaction: IQA perspective

Author(s): Badri, Z (Badri, Zahra); Foroutan-Nejad, C (Foroutan-Nejad, Cina); Kozelka, J (Kozelka, Jiri); Marek, R (Marek, Radek)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 17 **Issue:** 39 **Pages:** 26183-26190 **DOI:** 10.1039/c5cp04489h **Published:** 2015

Abstract: In the present work the nature of lone-pair-pi interactions between water molecules and a number of p-rings with different substituents/hetero-atoms in the light of quantum chemical topology approaches is studied. The Quantum Theory of Atoms in Molecules (QTAIM) and Interacting Quantum Atoms (IQA) were employed for distinguishing the role of heteroatoms and electron withdrawing substituents in the complex formation between water and p-rings. Our IQA study identified three classes of water-pi complexes on the basis of the relative role of electrostatics (classical) and exchange-correlation (non-classical) factors in the interaction energy between the oxygen of water (the lone-pair donor) and the sp(2) atoms of the p-ring, i.e. the primary lp-pi interaction. Considering both the primary and secondary (the rest of interatomic interactions except O-water-pi-ring atoms) interactions demonstrates that the exchange-correlation is the dominant contributor to the binding energy. This proves a non-negligible contribution of non-classical factors in the stabilization of the lone-pair-pi complexes. However, in spite of a relatively large contribution of the exchange-correlation, this part of the interaction energy is virtually counterbalanced by the deformation energy, i.e. the increase in atomic kinetic energy upon complexation. This finding clarifies why water-pi interactions can be modelled by simple electrostatics without the need to invoke quantum effects.

Accession Number: WOS:000362291300057
PubMed ID: 26381704
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173

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Record 483 of 491

Title: Aromatic Schiff Bases Multiply Substituted with Terminal Ethynyl Groups: Potential Building Blocks for Conjugated Polymers and Oligomers
Author(s): Stahlova, S (Stahlova, Sabina); Sedlacek, J (Sedlacek, Jan); Svoboda, J (Svoboda, Jan); Polasek, M (Polasek, Miroslav); Zednik, J (Zednik, Jiri)
Source: AUSTRALIAN JOURNAL OF CHEMISTRY **Volume:** 68 **Issue:** 8 **Pages:** 1237-1248 **DOI:** 10.1071/CH14639 **Published:** 2015
Abstract: Nine mostly novel aromatic Schiff bases containing from two-to-four terminal ethynyl groups and one or two methanimine groups per one molecule are reported. The spectral and density functional theory characteristics and the extent of conjugation are discussed in connection with the structure and architecture of the prepared compounds. The applicability of compounds as building blocks for conjugated polymers is shown in TaCl5-catalyzed polycyclotrimerization (proceeding in ethynyl groups) yielding either soluble luminescent or insoluble microporous polymers.
Accession Number: WOS:000359186700010
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sedlacek, Jan	F-3617-2014	0000-0002-6754-6628
Zednik, Jiri	F-2637-2014	0000-0001-7325-8684
Svoboda, Jan	E-4750-2014	0000-0002-4989-4274
Polasek, Miroslav	G-7217-2014	

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Record 484 of 491

Title: Correlation between the electronic structure, effective mass and thermoelectric properties of rare earth tellurides Ba2MYTe5 (M = Ga, In)
Author(s): Khan, W (Khan, Wilayat); Borek, S (Borek, Stephan); Minar, J (Minar, Jan)
Source: RSC ADVANCES **Volume:** 5 **Issue:** 64 **Pages:** 51461-51469 **DOI:** 10.1039/c5ra07678a **Published:** 2015
Abstract: Rare earth telluride compounds, namely Ba2MYTe5 (M = Ga, In), are the focus of this work due to their semiconducting nature, optoelectronic and thermoelectric properties. Their band gaps lie in the range of 1.08 to 1.36 eV, providing these compounds with opto- and thermo-electric properties. Here, we have studied the rare earth telluride single crystals of Ba2MYTe5 (M = Ga, In) using the full potential linearized augmented plane wave package WIEN2k. The direct band gaps were calculated using the modified Becke-Johnson approach which is in good agreement with the band gaps obtained from diffuse reflectance spectra. The density of states reveals a strong hybridization between Y 5s/4p, Ga 3d, Te 5p and Y 4d orbitals, indicative of covalent bonding. Besides, the electronic charge density contour discloses a mix of ionic and covalent bonding between the elements. We also report the thermoelectric properties studied through the temperature dependent electronic and thermal conductivities, as well as the Seebeck coefficient and the power factor using the BoltzTraP code.
Accession Number: WOS:000356305300001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Minar, Jan	O-3186-2013	0000-0001-9735-8479

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Record 485 of 491

Title: Slovak Economy in a Period of Recession: Nonlinear DSGE Model with Time-varying Parameters
Author(s): Tvrz, S (Tvrz, Stanislav); Vasicek, O (Vasicek, Osvald)
Source: EKONOMICKY CASOPIS **Volume:** 63 **Issue:** 1 **Pages:** 34-50 **Published:** 2015
Abstract: In this paper, we study the dramatic changes in the structure and behaviour of the Slovak economy in a period of the accession to the Euro area and the Great Recession and subsequent return to the long-run growth equilibrium. This small and very open economy is represented by nonlinear dynamic stochastic model of a general equilibrium with financial accelerator. The development of time-varying structural parameters is identified using the second order approximation of a nonlinear DSGE model. The model is estimated with the use of nonlinear particle filter. Analogous model was estimated for the economy of the Euro area. It is our goal to identify the most important changes in behaviour and underlying structure of the Slovak economy. In order to distinguish the country specific changes from broader Europe-wide trends we also compare the time-varying estimates of the Slovak economy and the Euro area.
Accession Number: WOS:000351890200003
ISSN: 0013-3035

Record 486 of 491

Title: Asymmetric bifurcated halogen bonds
Author(s): Novak, M (Novak, Martin); Foroutan-Nejad, C (Foroutan-Nejad, Cina); Marek, R (Marek, Radek)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 17 **Issue:** 9 **Pages:** 6440-6450 **DOI:** 10.1039/c4cp05532b **Published:** 2015
Abstract: Halogen bonding (XB) is being extensively explored for its potential use in advanced materials and drug design. Despite significant progress in describing this interaction by theoretical and experimental methods, the chemical nature remains somewhat elusive, and it seems to vary with the selected system. In this work we present a detailed DFT analysis of three-center asymmetric halogen bond (XB) formed between dihalogen molecules and variously 4-substituted 1,2-dimethoxybenzene. The energy decomposition, orbital, and electron density analyses suggest that the contribution of electrostatic stabilization is comparable with that of non-electrostatic factors. Both terms increase parallel with increasing negative charge of the electron donor molecule in our model systems. Depending on the orientation of the dihalogen molecules, this bifurcated interaction may be classified as 'sigma-hole - lone pair' or 'sigma-hole - pi' halogen bonds. Arrangement of the XB investigated here deviates significantly from a recent IUPAC definition of XB and, in analogy to the hydrogen bonding, the term bifurcated halogen bond (BXB) seems to be appropriate for this type of interaction.
Accession Number: WOS:000351435300032
PubMed ID: 25656525
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Novak, Martin	I-3248-2015	0000-0001-5067-1994

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Record 487 of 491

Title: Magnetorotational instability in decretion disks of critically rotating stars and the outer structure of Be and Be/X-ray disks
Author(s): Krticka, J (Krticka, J.); Kurfurst, P (Kurfuerst, P.); Krtickova, I (Krtickova, I.)
Source: ASTRONOMY & ASTROPHYSICS **Volume:** 573 **Article Number:** A20 **DOI:** 10.1051/0004-6361/201424867 **Published:** JAN 2015
Abstract: Context. Evolutionary models of fast-rotating stars show that the stellar rotational velocity may approach the critical speed. Critically rotating stars cannot spin up more, therefore they lose their excess angular momentum through an equatorial outflowing disk. The radial extension of such disks is unknown, partly because we lack information about the radial variations of the viscosity.
Aims. We study the magnetorotational instability, which is considered to be the origin of anomalous viscosity in outflowing disks.

Methods. We used analytic calculations to study the stability of outflowing disks submerged in the magnetic field.
Results. The magnetorotational instability develops close to the star if the plasma parameter is large enough. At large radii the instability disappears in the region where the disk orbital velocity is roughly equal to the sound speed.
Conclusions. The magnetorotational instability is a plausible source of anomalous viscosity in outflowing disks. This is also true in the region where the disk radial velocity approaches the sound speed. The disk sonic radius can therefore be roughly considered as an effective outer disk radius, although disk material may escape from the star to the insterstellar medium. The radial profile of the angular momentum-loss rate already flattens there, consequently, the disk mass-loss rate can be calculated with the sonic radius as the effective disk outer radius. We discuss a possible observation determination of the outer disk radius by using Be and Be/X-ray binaries.

Accession Number: WOS:000346901300087

ISSN: 1432-0746

Record 488 of 491

Title: Functional helquats: helical cationic dyes with marked, switchable chiroptical properties in the visible region

Author(s): Reyes-Gutierrez, PE (Reyes-Gutierrez, Paul E.); Jirasek, M (Jirasek, Michael); Severa, L (Severa, Lukas); Novotna, P (Novotna, Pavlina); Koval, D (Koval, Dusan); Sazelova, P (Sazelova, Petra); Vavra, J (Vavra, Jan); Meyer, A (Meyer, Andreas); Cisarova, I (Cisarova, Ivana); Saman, D (Saman, David); Pohl, R (Pohl, Radek); Stepanek, P (Stepanek, Petr); Slavicek, P (Slavicek, Petr); Coe, BJ (Coe, Benjamin J.); Hajek, M (Hajek, Miroslav); Kasicka, V (Kasicka, Vaclav); Urbanova, M (Urbanova, Marie); Teply, F (Teply, Filip)

Source: CHEMICAL COMMUNICATIONS **Volume:** 51 **Issue:** 9 **Pages:** 1583-1586 **DOI:** 10.1039/c4cc08967g **Published:** 2015

Abstract: Helquat dyes are the first helicene-like cationic styryl dyes obtained as separate enantiomers. Their remarkable chiroptical properties are due to the unique combination of a cationic hemicyanine chromophore and a helicene-like motif. The magnitude of the ECD response and the pH switching along with their positioning in the visible region are unprecedented among helicenoids.

Accession Number: WOS:000348200100005

PubMed ID: 25555172

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koval, Dusan	G-5432-2014	0000-0002-6424-3891
Cisarova, Ivana	B-1385-2017	0000-0002-9612-9831
Stepanek, Petr	G-7636-2014	0000-0001-5000-8180
Slavicek, Petr	B-7511-2008	
Reyes Gutierrez, Paul Eduardo	D-5606-2013	0000-0002-6325-8936
Urbanova, Marie	E-4286-2014	
Severa, Lukas	G-6486-2014	
Hajek, Miroslav	G-1364-2014	0000-0002-8906-243X
Teply, Filip		0000-0003-3459-556X
Meyer, Andreas		0000-0002-8650-1847

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Record 489 of 491

Title: Species interactions during diversification and community assembly in Malagasy Miniopterus bats

Author(s): Schoeman, MC (Schoeman, M. Corrie); Goodman, SM (Goodman, Steven M.); Ramasindrazana, B (Ramasindrazana, Beza); Koubinova, D (Koubinova, Darina)

Source: EVOLUTIONARY ECOLOGY **Volume:** 29 **Issue:** 1 **Pages:** 17-47 **DOI:** 10.1007/s10682-014-9745-4 **Published:** JAN 2015

Abstract: The habitat first rule (HFR) proposes that radiating species initially diversify into habitat specialists and later into dietary specialists within a given habitat, whereas the general vertebrate model (GVM) adds divergence of sexually selected traits as a possible third axis of specialization subsequent to habitat and dietary divergence. In this study, using 12 Miniopterus spp. from Madagascar we test predictions of the HFR and GVM from ecological and evolutionary perspectives on Grinnellian and Eltonian niche structures. We used environmental niche models (ENMs) to quantify the Grinnellian niche, both for current and last inter-glacial climates. We used null models to examine Eltonian niche patterns of sympatric species in terms of their phylogenetic relatedness and phenotypic and sensory characters associated with the trophic niche-body size, skull morphology and echolocation. As predicted by the HFR, we found evidence for labile Grinnellian niches: there was no similarity in ENMs between sister species; overlap in ENMs was significantly low in > 65 % of all possible species pairs; there was no relationship between ENM niche overlap and phylogenetic distances between species; and there was no phylogenetic signal in suitable bioclimatic zones among species. Conversely, we found equivocal support for the HFR regarding Eltonian niche patterns. Closely related species tended to be distributed among ensembles rather than within ensembles, although there was no evidence for overdispersion in phylogenetic patterns in ensembles. In < 50 % of the observed combinations of sympatric Miniopterus spp., we found significant signal for overdispersion of phenotypic and sensory characters. We hypothesize that selective processes associated with the adaptive radiation of Miniopterus spp. on Madagascar may have favoured bats to diversify first into broad scale habitat specialists, but argue that understanding the relative influence of bionomic processes at a local spatial scale will require more reciprocal comparisons of Eltonian niches.

Accession Number: WOS:000347528300002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Koubinova, Darina	M-6157-2013	0000-0002-1854-7675
Schoeman, Corrie	G-2616-2010	

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Record 490 of 491

Title: N-acyl-omega-aminoaldehydes are efficient substrates of plant aminoaldehyde dehydrogenases

Author(s): Frommel, J (Froemmel, Jan); Sebela, M (Sebela, Marek); Demo, G (Demo, Gabriel); Lenobel, R (Lenobel, Rene); Pospisil, T (Pospisil, Tomas); Soural, M (Soural, Miroslav); Kopecny, D (Kopecny, David)

Source: AMINO ACIDS **Volume:** 47 **Issue:** 1 **Pages:** 175-187 **DOI:** 10.1007/s00726-014-1853-5 **Published:** JAN 2015

Abstract: Plant aminoaldehyde dehydrogenases (AMADHs, EC 1.2.1.19) belong to the family 10 of aldehyde dehydrogenases and participate in the metabolism of compounds related to amino acids such as polyamines or osmoprotectants. Their broad specificity covers omega-aminoaldehydes, aliphatic and aromatic aldehydes as well as nitrogen-containing heterocyclic aldehydes. The substrate preference of plant AMADHs is determined by the presence of aspartic acid and aromatic residues in the substrate channel. In this work, 15 new N-acyl derivates of 3-aminopropanal (APAL) and 4-aminobutanal (ABAL) were synthesized and confirmed as substrates of two pea AMADH isoenzymes (PsAMADH 1 and 2). The compounds were designed considering the previously demonstrated conversion of N-acetyl derivatives as well as substrate channel dimensions (5-8 x 14). The acyl chain length and its branching were found less significant for substrate properties than the length of the initial natural substrate. In general, APAL derivatives were found more efficient than the corresponding ABAL derivatives because of the prevailing higher conversion rates and lower K (m) values. Differences in enzymatic performance between the two isoenzymes corresponded in part to their preferences to APAL to ABAL. The higher PsAMADH2 affinity to substrates correlated with more frequent occurrence of an excess substrate inhibition. Molecular docking indicated the possible auxiliary role of Tyr163, Ser295 and Gln451 in binding of the new substrates. The only derivative carrying a free carboxyl group (N-adipoyl APAL) was surprisingly better substrate than ABAL in PsAMADH2 reaction indicating that also negatively charged aldehydes might be good substrates for ALDH10 family.

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PubMed ID: 25344796

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Demo, Gabriel	D-7261-2012	0000-0002-5472-9249
Pospisil, Tomas		0000-0003-3634-828X
Kopecny, David		0000-0002-4309-4284

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Record 491 of 491

Title: HPS: High precision stemmer

Author(s): Brychcin, T (Brychcin, Tomas); Konopik, M (Konopik, Miloslav)

Source: INFORMATION PROCESSING & MANAGEMENT **Volume:** 51 **Issue:** 1 **Pages:** 68-91 **DOI:** 10.1016/j.ipm.2014.08.006 **Published:** JAN 2015

Abstract: Research into unsupervised ways of stemming has resulted, in the past few years, in the development of methods that are reliable and perform well. Our approach further shifts the boundaries of the state of the art by providing more accurate stemming results. The idea of the approach consists in building a stemmer in two stages. In the first stage, a stemming algorithm based upon clustering, which exploits the lexical and semantic information of words, is used to prepare large-scale training data for the second-stage algorithm. The second-stage algorithm uses a maximum entropy classifier. The stemming-specific features help the classifier decide when and how to stem a particular word.
In our research, we have pursued the goal of creating a multi-purpose stemming tool. Its design opens up possibilities of solving non-traditional tasks such as approximating lemmas or improving language modeling. However, we still aim at very good results in the traditional task of information retrieval. The conducted tests reveal exceptional performance in all the above mentioned tasks. Our stemming method is compared with three state-of-the-art statistical algorithms and one rule-based algorithm. We used corpora in the Czech, Slovak, Polish, Hungarian, Spanish and English languages. In the tests, our algorithm excels in stemming previously unseen words (the words that are not present in the training set). Moreover, it was discovered that our approach demands very little text data for training when compared with competing unsupervised algorithms. (C) 2014 Elsevier Ltd. All rights reserved.

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Author Identifiers:

Author	ResearcherID Number	ORCID Number
Brychcin, Tomas	C-1181-2016	0000-0002-7442-0978

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