Record 1 of 214

Title: Roughness of Transmembrane Helices Reduces Lipid Membrane Dynamics

Author(s): Olsinova, M (Olsinova, Marie); Jurkiewicz, P (Jurkiewicz, Piotr); Kishko, I (Kishko, Iryna); Sykora, J (Sykora, Jan); Sabo, J (Sabo, Jan); Hof, M (Hof, Martin); Cwiklik, L (Cwiklik, Lukasz); Cebecauer, M (Cebecauer, Marek)

Source: ISCIENCE **Volume:** 10 **Pages:** 87-+ **DOI:** 10.1016/j.isci.2018.11.026 **Published:** DEC 21 2018

Abstract: The dynamics of cellular membranes is primarily determined by lipid species forming a bilayer. Proteins are considered mainly as effector molecules of diverse cellular processes. In addition to large assemblies of proteins, which were found to influence properties of fluid membranes, biological membranes are densely populated by small, highly mobile proteins. However, little is known about the effect of such proteins on the dynamics of membranes. Using synthetic peptides, we demonstrate that transmembrane helices interfere with the mobility of membrane components by trapping lipid acyl chains on their rough surfaces. The effect is more pronounced in the presence of cholesterol, which segregates from the rough surface of helical peptides. This may contribute to the formation or stabilization of membrane heterogeneities. Since roughness is a general property of helical transmembrane segments, our results suggest that, independent of their size or cytoskeleton linkage, integral membrane proteins affect local membrane dynamics and organization.

Accession Number: WOS:000454331700008

PubMed ID: 30508721

ISSN: 2589-0042

Record 2 of 214

Title: Shape-selective crystallisation of fluxional carbon cages

Author(s): Bismillah, AN (Bismillah, Aisha N.); Sturala, J (Sturala, Jiri); Chapin, BM (Chapin, Brette M.); Yufit, DS (Yufit, Dmitry S.); Hodgkinson, P (Hodgkinson, Paul); McGonigal, PR (McGonigal, Paul R.)

Source: CHEMICAL SCIENCE **Volume:** 9 **Issue:** 46 **DOI:** 10.1039/c8sc04303e **Published:** DEC 14 2018

Abstract: Dynamic covalent rearrangements of fluxional carbon cages, such as bullvalenes and barbaralanes, impart shapeshifting' molecular properties. Here, a series of five barbaralanes each interconvert dynamically between two constitutional isomers in solution, but resolve to single isomers upon crystallisation. Unexpectedly, the minor solution-phase isomers are resolved in two instances. Through dynamic NMR, crystallographic and DFT analyses, we show that the isomer observed in the solid state is not a direct consequence of the equilibrium distribution in solution or any specific noncovalent interactions. Rather, the dynamic preferential crystallisation is dictated by differences in molecular size and shape.

Accession Number: WOS:000451533000001

ISSN: 2041-6520

eISSN: 2041-6539

Record 3 of 214

Title: Dynamics of multiple protoplanets embedded in gas and pebble discs and its dependence on Sigma and nu parameters

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

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 620 **Article Number:** A157 **DOI:** 10.1051/0004-6361/201833855 **Published:** DEC 12 2018

Abstract: Protoplanets of super-Earth size may get trapped in convergence zones for planetary migration and form gas giants there. These growing planets undergo accretion heating, which triggers a hot-trail effect that can reverse migration directions, increase planetary eccentricities, and prevent resonant captures of migrating planets. In this work, we study populations of embryos that are accreting pebbles under different conditions, by changing the surface density, viscosity, pebble flux, mass, and the number of protoplanets. For modelling, we used the FARGO-THORIN two-dimensional (2D) hydrocode, which incorporates a pebble disc as a second pressureless fluid, the coupling between the gas and pebbles, and the flux-limited diffusion approximation for radiative transfer. We find that massive embryos embedded in a disc with high surface density (Sigma = 990 g cm(-2) at 5.2 au) undergo numerous "unsuccessful" two-body encounters that do not lead to a merger. Only when a third protoplanet arrives in the convergence zone do three-body encounters lead to mergers. For a low-viscosity disc (nu = 5 x 10(13) cm(2) s(-1)), a massive co-orbital is a possible outcome, for which a pebble isolation develops and the co-orbital is further stabilised. For more massive protoplanets (5 M-circle plus), the convergence radius is located further out, in the ice-giant zone. After a series of encounters, there is an evolution driven by a dynamical torque of a tadpole region, which is systematically repeated several times until the co-orbital configuration is disrupted and planets merge. This may be a way to solve the problem that co-orbitals often form in simulations but they are not observed in nature. In contrast, the joint evolution of 120 low-mass protoplanets (0.1 M-circle plus) reveals completely different dynamics. The evolution is no longer smooth, but rather a random walk. This is because the spiral arms, developed in the gas disc due to Lindblad resonances, overlap with each other and affect not only a single protoplanet but several in the surrounding area. Our hydrodynamical simulations may have important implications for N-body simulations of planetary migration that use simplified torque prescriptions and are thus unable to capture protoplanet dynamics in its full glory.

Accession Number: WOS:000452879800002

ISSN: 1432-0746

Record 4 of 214

Title: Brilliant gamma-ray beam and electron-positron pair production by enhanced attosecond pulses

Author(s): Gu, YJ (Gu, Yan-Jun); Klimo, O (Klimo, Ondrej); Bulanov, SV (Bulanov, Sergei, V); Weber, S (Weber, Stefan)

Source: COMMUNICATIONS PHYSICS **Volume:** 1 **Article Number:** 93 **DOI:** 10.1038/s42005-018-0095-3 **Published:** DEC 10 2018

Abstract: Electron-positron pair production via Breit-Wheeler process requires laser intensities approaching 10(24) W cm(-2) due to the small cross-section. Here, we propose a mechanism for brilliant gamma-ray emission and dense GeV pairs creation accompanied with high-harmonic generation by using plasma mirror and an ultra short pulse with the intensity of 3 x 10(23) W cm(-2). The laser is reflected by the solid surface after propagating tens of microns in a near-critical density plasma and breaks into short wave packets. The intensity of the reflected high order harmonic field is enhanced by the focusing and compression effects from the deformed oscillating mirror. The radiation trapped electrons emit gamma-photons while colliding with the reflected attosecond pulses. The peak intensity of the gamma-ray reaches 0.74 PW with the brilliance of 2 x 10(24) s(-1) mm(-2) mrad(-2) (0.1%BW)(-1) (at 58 MeV). A GeV positron beam is obtained with density of 4 x 10(21) cm(-3) and a particle number of 5.6 x 10(9).

Accession Number: WOS:000452676600001

ISSN: 2399-3650

Record 5 of 214

Title: Facile Construction and In Silico Study of Quinoline-Attached Resorcinarene Fluorescent Sensor for the Recognition of Insensitive Munition Compounds

Author(s): Panchal, U (Panchal, Urvi); Modi, K (Modi, Krunal); Liska, A (Liska, Alan); Ludvik, J (Ludvik, Jiri); Dey, S (Dey, Shuvankar); Patel, C (Patel, Chirag); Jain, VK (Jain, V. K.)

Source: CHEMISTRYSELECT **Volume:** 3 **Issue:** 45 **Pages:** 12951-12959 **DOI:** 10.1002/slct.201802586 **Published:** DEC 6 2018

Abstract: N-methyl-4-nitroaniline (MNA), an insensitive munition is selectively and sensitively recognized by a new resorcinarene bearing quinoline moiety, i.e, Tetra-Methoxy Resorcinarene Tetra-Quinoline Acetamide (TMRTQA). A simple and efficient spectrofluorimetric technique demonstrates the quenching of the fluorescence intensity of TMRTQA upon addition of MNA within concentration limits of 2 nM to 1 mu M. Binding constant and quantum yield have been determined in this study. Molecular docking studies have been performed to predict the best binding affinity and the possible interactions for the formation of complex between TMRTQA and MNA supporting the 1:1 stoichiometry. Density functional theory calculation also support the excitation wavelength and geometry optimization. MNA being a hazardous environmental pollutant has been successfully detected from the water sample by standard addition method.

Accession Number: WOS:000452260800030

ISSN: 2365-6549

Record 6 of 214

Title: Identification and partial characterization of a novel serpin from Eudiplozoon nipponicum (Monogenea, Polyopisthocotylea)

Author(s): Roudnicky, P (Roudnicky, Pavel); Vorel, J (Vorel, Jiri); Ilgova, J (Ilgova, Jana); Benovics, M (Benovics, Michal); Norek, A (Norek, Adam); Jedlickova, L (Jedlickova, Lucie); Mikes, L (Mikes, Libor); Potesil, D (Potesil, David); Zdrahal, Z (Zdrahal, Zbynek); Dvorak, J (Dvorak, Jan); Gelnar, M (Gelnar, Milan); Kasny, M (Kasny, Martin)

Source: PARASITE **Volume:** 25 **Article Number:** 61 **DOI:** 10.1051/parasite/2018062 **Published:** DEC 5 2018

Abstract: Background: Serpins are a superfamily of serine peptidase inhibitors that participate in the regulation of many physiological and cell peptidase-mediated processes in all organisms (e.g. in blood clotting, complement activation, fibrinolysis, inflammation, and programmed cell death). It was postulated that in the blood-feeding members of the monogenean family Diplozoidae, serpins could play an important role in the prevention of thrombus formation, activation of complement, inflammation in the host, and/or in the endogenous regulation of protein degradation.

Results: In silico analysis showed that the DNA and primary protein structures of serpin from Eudiplozoon nipponicum (EnSerp1) are similar to other members of the serpin superfamily. The inhibitory potential of EnSerp1 on four physiologically-relevant serine peptidases (trypsin, factor Xa, kallikrein, and plasmin) was demonstrated and its presence in

the worm's excretory-secretory products (ESPs) was confirmed.

Conclusion: EnSerp1 influences the activity of peptidases that play a role in blood coagulation, fibrinolysis, and complement activation. This inhibitory potential, together with the serpin's presence in ESPs, suggests that it is likely involved in host-parasite interactions and could be one of the molecules involved in the control of feeding and prevention of inflammatory responses.

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PubMed ID: 30516130

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ISSN: 1252-607X

eISSN: 1776-1042

Record 7 of 214

Title: Saturated aqueous NaCl solution and pure water in Na-montmorillonite clay at thermodynamic conditions of hydraulic fracturing: Thermodynamics, structure and diffusion from molecular simulations

Author(s): Svoboda, M (Svoboda, Martin); Moucka, F (Moucka, Filip); Lisal, M (Lisal, Martin)

Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 271 **Pages:** 490-500 **DOI:** 10.1016/j.molliq.2018.08.144 **Published:** DEC 1 2018

Abstract: We present a Grand Canonical Monte Carlo (GCMC) and molecular dynamics (MD) simulation study of an aqueous NaCl solution in Na-montmorillonite (Na-MMT) clay pores, including the thermodynamic, structural and dynamical properties. We represent the clay pores by Na-MMT slits of an interlayer separation ranging from about 10 to 32 angstrom, covering clay pores from dry clay to clay pores with a bulk-like water layer in the middle of the pore. We consider the clay in equilibrium with the saturated salt solution at a typical shale gas reservoir condition of a temperature of 365K and a pressure of 275 bar. The equilibrium amount of the adsorbed ions and water molecules obtained from the GCMC simulations are employed in MD to simulate the disjoining pressure and in turn the swelling free energy curve which determines the number of stable states in the clay, their composition, and the corresponding equilibrium interlayer separations. In addition, using MD simulations, we evaluate the hydration energy, atomic and charge density profiles, orientation distribution, hydrogen-bond network, and in-plane self-diffusivity of the water and ions to provide insight into the microscopic behaviour of the aqueous NaCl solution in the interlayer galleries of the hydrophilic Na-MMT pores. We compare the simulation results for the confined aqueous NaCl solutions with those obtained for the Na-MMT in equilibrium with a pure water reservoir at the same temperature and pressure. (C) 2018 Elsevier B.V. All rights reserved.

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Record 8 of 214

Title: High-throughput amplicon sequencing-based analysis of active fungal communities inhabiting grapevine after hot-water treatments reveals unexpectedly high fungal diversity

Author(s): Eichmeier, A (Eichmeier, Ales); Pecenka, J (Pecenka, Jakub); Penazova, E (Penazova, Eliska); Baranek, M (Baranek, Miroslav); Catala-Garcia, S (Catala-Garcia, Santiago); Leon, M (Leon, Maela); Armengol, J (Armengol, Josep); Gramaje, D (Gramaje, David)

Source: FUNGAL ECOLOGY **Volume:** 36 **Pages:** 26-38 **DOI:** 10.1016/j.funeco.2018.07.011 **Published:** DEC 2018

Abstract: The ecology of total fungal communities in grapevine is so far largely derived from studies on culture-dependent methods or cultivation-independent rDNA approaches. Sequencing the ribosomal RNA transcripts (rRNA) would rather reveal the functionally and metabolically active important taxa of the fungal community and provide insights into its activity in the wood. The present study investigated changes in the potentially active fungal communities of internal grapevine wood after Hot-Water Treatment (HWT) in planting material from Czech Republic and Spain at two different times during the propagation process and from two plant zones. We examined fungal communities using both traditional isolation into culture and high-throughput amplicon sequencing (HTAS) of the internal transcribed spacer 2 (ITS2) region in extracted total RNA. HTAS from metatranscriptomic RNA increased the resolution of the fungal community analysis and revealed a highly diverse mycobiota of grapevine wood compared to the traditional method. Fungal diversity differed between grapevine genotypes and showed a temporal variation over the vegetative period. Grapevine planting materials exhibited high fungal diversity after HWT, which demonstrates that the HWT process does not sterilize the internal wood of grapevine. HWT reduced the infection caused by fungal trunk disease pathogens but was not completely effective in eliminating their growth. This study provides important and practically useful insights into the dynamics of active fungal communities in hot-water treated plants, and represents the first study of active fungal communities on grapevine grafted plants by comparing traditional and next-generation sequencing methods. (C) 2018 Elsevier Ltd and British Mycological Society. All rights reserved.

Accession Number: WOS:000452564900004

ISSN: 1754-5048

eISSN: 1878-0083

Record 9 of 214

Title: Binary Planet Formation by Gas-assisted Encounters of Planetary Embryos

Author(s): Chrenko, O (Chrenko, Ondrej); Broz, M (Broz, Miroslav); Nesvorny, D (Nesvorny, David)

Source: ASTROPHYSICAL JOURNAL **Volume:** 868 **Issue:** 2 **Article Number:** 145 **DOI:** 10.3847/1538-4357aaeb93 **Published:** DEC 1 2018

Abstract: We present radiation hydrodynamic simulations in which binary planets form by close encounters in a system of several super-Earth embryos. The embryos are embedded in a protoplanetary disk consisting of gas and pebbles and evolve in a region where the disk structure supports convergent migration due to Type I torques. As the embryos accrete pebbles, they become heated and thus affected by the thermal torque and the hot-trail effect, which excites orbital eccentricities. Motivated by findings of Eklund & Masset, we assume that the hot-trail effect also operates vertically and reduces the efficiency of inclination damping. Non-zero inclinations allow the embryos to become closely packed and also vertically stirred within the convergence zone. Subsequently, close encounters of two embryos assisted by the disk gravity can form transient binary planets that quickly dissolve. Binary planets with a longer lifetime of similar to 10(4) yr form in three-body interactions of a transient pair with one of the remaining embryos. The separation of binary components generally decreases in subsequent encounters and because of pebble accretion until the binary merges, forming a giant planet core. We provide an order-of-magnitude estimate of the expected occurrence rate of binary planets, yielding one binary planet per similar or equal to(2-5) x 10(4) planetary systems. Therefore, although rare, binary planets may exist in exoplanetary systems and they should be systematically searched for.

Accession Number: WOS:000452414800003

ISSN: 0004-637X

eISSN: 1538-4357

Record 10 of 214

Title: The Safety Control Of The Electrical Stimulation Mapping Using Numerical Simulation

Author(s): Janca, R (Janca, R.); Vrba, J (Vrba, J.); Vrba, D (Vrba, D.); Blaha, M (Blaha, M.); Jezdik, P (Jezdik, P.); Jahodova, A (Jahodova, A.); Kudr, M (Kudr, M.); Komarek, V (Komarek, V.); Krsek, P (Krsek, P.)

Source: EPILEPSIA **Meeting Abstract:** p495 **Volume:** 59 **Special Issue:** SI **Pages:** S226-S226 **Supplement:** 3 **Published:** DEC 2018

Accession Number: WOS:000451817900477

Conference Title: 13th European Congress on Epileptology

Conference Date: AUG 26-30, 2018

Conference Location: Vienna, AUSTRIA

ISSN: 0013-9580

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Record 11 of 214

Title: Electronic structure and thermoelectric properties of PbS1-Te-x(x) (x=0, 0.25, 0.50, 0.75, 1.0) alloys: Ab initio study

Author(s): Khan, SA (Khan, Saleem Ayaz); Azam, S (Azam, Sikander)

Source: SUPERLATTICES AND MICROSTRUCTURES **Volume:** 124 **Pages:** 248-256 **DOI:** 10.1016/j.spmi.2018.04.031 **Published:** DEC 2018

Abstract: We present electronic structure and thermoelectric behavior for the PbS1-Te-x(x) (x=0, 0.25, 0.50, 0.75, 1.0) using all electron full potential linearized augmented plane wave (FP-LAPW) method. The correct value of the band gap is achieved with fully relativistic calculation by employing spin orbit coupling to the Hamiltonian implicitly. Our study shows the interactions between Pb-s, Te-p and S-p states that play a leading role in the valance band while the Pb-p and S-p and Te-p states play a dominant role in conduction band. The thermoelectric properties discuss the variation of the electrical and thermal conductivity, Seebeck coefficient, power factor and figure of merit with temperature variation using the Boltzmann transport theory. The high-temperature figure of merit of Te doped PbS alloy have been found to be significantly greater than PbS. This improvement is associated to the ability to attain higher doping and, hence, larger electrical properties at high temperatures. Hence, it reveals that both PbS0.25Te0.75 and PbTe can be used as promising materials for

Accession Number: WOS:000449903200027
ISSN: 0749-6036

Record 12 of 214
Title: Higher virial coefficients of water
Author(s): Rouha, M (Rouha, Michael); Nezbeda, I (Nezbeda, Ivo); Hruby, J (Hruby, Jan); Moucka, F (Moucka, Filip)
Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 270 **Special Issue:** SI **Pages:** 81-86 **DOI:** 10.1016/j.molliq.2017.11.105 **Published:** NOV 15 2018
Abstract: Virial coefficients B-2 to B-4 for the non-polarizable TIP4P/2005 model of water and the polarizable BK3 model were computed. An analysis and assessment of available experimental and pseudoexperimental data is carried out. Various forms of the virial expansion are examined with respect to their potential use for the description of steam (working agent in turbines). At higher temperatures (higher densities) the expansion starts exhibiting an irregular behavior indicating that at these conditions the vapor can likely not be viewed as a system made up only of individual molecules, and the occurrence of clusters of different size must be accounted for. (C) 2017 Elsevier B.V. All rights reserved.
Accession Number: WOS:000451360200011
ISSN: 0167-7322
eISSN: 1873-3166

Record 13 of 214
Title: Temperature Dependence of Carbon Monoxide Adsorption on a High-Silica H-FER Zeolite
Author(s): Rubes, M (Rubes, Miroslav); Trachta, M (Trachta, Michal); Koudelkova, E (Koudelkova, Eva); Bulanek, R (Bulanek, Roman); Klimes, J (Klimes, Jiri); Nachtigall, P (Nachtigall, Petr); Bludsky, O (Bludsky, Ota)
Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 122 **Issue:** 45 **Pages:** 26088-26095 **DOI:** 10.1021/acs.jpcc.8b08935 **Published:** NOV 15 2018
Abstract: The temperature dependence of the isosteric heat of the CO adsorption on a high-silica protonic ferrierite (H-FER) zeolite was investigated using microcalorimetry and density functional theory/coupled-cluster (DFT/CC) atomistic simulations. A large change in the experimental heat of adsorption was observed at the zero-coverage limit for the CO/H-FER system (from 32.2 kJ/mol at 200 K to 25.4 kJ/mol at 300 K). This can be explained by a dramatic change in the CO dynamics in the 200-300 K temperature range. During our ab initio molecular dynamics simulation at 200 K, the CO molecule is localized; at 300 K, the molecule jumps between adjacent Bronsted sites. The only exception has been found for the T-4 '' site, where the fast desorption of the CO molecule is prevented by a curved ferrierite wall enclosing this site. The previously reported variable temperature adsorption of the CO/H-FER with Si/A1 27.5 (28.4(+/- 2) kJ/mol) is consistent with the Perdew-Burke-Ernzerhof/CC predictions for individual sites when the statistical distribution of adsorption sites and temperature effects are taken into account.
Accession Number: WOS:000451101400040
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Record 14 of 214
Title: Treatment of Herzberg-Teller and non-Condon effects in optical spectra with Hierarchical Equations of Motion
Author(s): Seibt, J (Seibt, Joachim); Mancal, T (Mancal, Tomas)
Source: CHEMICAL PHYSICS **Volume:** 515 **Pages:** 129-140 **DOI:** 10.1016/j.chemphys.2018.08.026 **Published:** NOV 14 2018
Abstract: We derive a Hierarchical Equations of Motion (HEOM) description of nonadiabatic Herzberg-Teller type coupling effects and of non-Condon effects in a system of electronic transitions interacting with intra- and inter-molecular vibrational modes. We point out analogies between the auxiliary density operators (ADOs) of the hierarchy and the terms arising from explicit description of the vibrational modes in the Hamiltonian. In comparison with the standard formulation of HEOM, our equations contain additional connections between ADOs in the hierarchy scheme, which account for the dependence of the nonadiabatic coupling elements on the vibrational coordinates. We compare absorption spectra calculated with our HEOM methodology and with explicit treatment of vibrational DOF for a dimer system in the strong resonance coupling regime. Furthermore, we show that for sufficiently strong excitonic coupling, the corresponding effects in linear absorption spectra of vibronic dimers can be captured very well by the concept of effective Huang-Rhys factors.
Accession Number: WOS:000454412800016
ISSN: 0301-0104
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Record 15 of 214
Title: Local versus global aromaticity in azuliporphyrin and benziporphyrin derivatives
Author(s): Ghosh, A (Ghosh, Abhik); Larsen, S (Larsen, Simon); Conradie, J (Conradie, Jeanet); Foroutan-Nejad, C (Foroutan-Nejad, Cina)
Source: ORGANIC & BIOMOLECULAR CHEMISTRY **Volume:** 16 **Issue:** 42 **Pages:** 7964-7970 **DOI:** 10.1039/c8ob01672k **Published:** NOV 14 2018
Abstract: Carbaporphyrinoids afford fascinating examples of competition between local and global aromaticity in conjugated, polycyclic systems. Thus, whereas density functional theory calculations reveal only a modest effect of metal complexation on the current density profiles of true carbaporphyrins and azuliporphyrins, the impact is much greater for benziporphyrins, underscoring a strong competition between local and global aromaticity in the latter system. Furthermore, the calculations shed light on the remarkable efficacy of suitably placed electron-donating substituents on the benzene ring in boosting the global diatropic currents in a metallobenziporphyrin.
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PubMed ID: 30325395
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ISSN: 1477-0520
eISSN: 1477-0539

Record 16 of 214
Title: Radiative Charge Transfer between Metastable Helium and Lithium Cations
Author(s): Zamecnikova, M (Zamecnikova, Martina); Kraemer, WP (Kraemer, Wolfgang P.); Soldan, P (Soldan, Pavel)
Source: ASTROPHYSICAL JOURNAL **Volume:** 867 **Issue:** 2 **Article Number:** 157 **DOI:** 10.3847/1538-4357/aae64f **Published:** NOV 10 2018
Abstract: Depopulation of long-lived metastable helium He(2(3)S) by spontaneous radiative charge transfer in collisions with lithium cations Li+ is investigated using a fully quantal approach. The corresponding transitions start in continuum states of the initial electronic state b(3)Sigma(+) and end in continuum states of the final electronic state a(3)Sigma(+). The process is characterized by cross sections and rate coefficients, which are calculated as functions of initial collision energy and temperature, respectively. Particular consideration is paid to the proper description of the high-energy cross sections in order to include their contributions to the total rate coefficient at high temperatures, where its asymptotic behavior is analyzed. The calculated total rate coefficients are in the range 1.75 x 10(-15) - 3.16 x 10(-14) cm(3) s(-1). The comparison with other relevant depopulation mechanisms shows that the radiative processes prevail for temperatures below 3000 K, while at higher temperatures the nonradiative inelastic processes are dominant.
Accession Number: WOS:000450221700024
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ISSN: 0004-637X
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Record 17 of 214
Title: Rational design of sensor for broadband dielectric spectroscopy of biomolecules
Author(s): Havelka, D (Havelka, Daniel); Krivosudsky, O (Krivosudsky, Ondrej); Prusa, J (Prusa, Jiri); Cifra, M (Cifra, Michal)

Abstract: Knowledge of electromagnetic properties of biomolecules is essential for a fundamental understanding of electric field interaction with biosystems and for development of novel biomedical diagnostic and therapeutic methods. To enable systematic analysis of the dielectric properties of biomolecule solutions we presented here a method for a rational design of radiofrequency and microwave chip for quantitative dielectric sensing. At first, we estimated the primary frequency band of interest using a relaxation time of targeted molecule via the Stokes-Einstein-Debye equation. Then we proposed a microwave sensing chip for the estimated frequency band and evaluated its performance using both analytical modeling and numerical electromagnetic simulations. We fabricated the chip and experimentally demonstrated that we can extract the complex permittivity (0.5-40 GHz) of the water solution of alanine - one of the most common proteinogenic amino acids - without any calibration liquid and with about 20-fold smaller volume than with commercial methods. The observed dependence of extracted complex permittivity on the alanine concentration was interpreted using molecular dynamics simulations. The procedure we described here can be applied for the development of dielectric sensing method of any polar biomolecule solution.

Record 18 of 214
Title: Slicing conditions for axisymmetric gravitational collapse of Brill waves

Author(s): Khirnov, A (Khirnov, Anton); Ledvinka, T (Ledvinka, Tomas)

Abstract: In numerical relativity, spacetimes involving compact strongly gravitating objects are constructed as numerical solutions of Einstein's equations. Success of such a process strongly depends on the availability of appropriate coordinates, which are typically constructed dynamically. A very robust coordinate choice is a so-called moving puncture gauge, commonly used for numerical simulations of black hole spacetimes. Nevertheless it is known to fail for evolving near-critical Brill wave data. We construct a new 'quasi-maximal' slicing condition and demonstrate that it exhibits better behavior for such data. This condition is based on the 1+log slicing with an additional source term derived from maximal slicing. It is relatively simple to implement in existing moving puncture codes and computationally inexpensive. We also illustrate the properties of constructed spacetimes based on gauge-independent quantities in compactified spacetime diagrams. These invariants are also used to show how created black holes settle down to a Schwarzschild black hole.

Record 19 of 214
Title: Domestic Fowl Breed Variation in Egg White Protein Expression: Application of Proteomics and Transcriptomics

Author(s): Bilkova, B (Bilkova, Barbora); Swiderska, Z (Swiderska, Zuzana); Zita, L (Zita, Lukas); Laloe, D (Laloe, Denis); Charles, M (Charles, Mathieu); Benes, V (Benes, Vladimir); Stopka, P (Stopka, Pavel); Vinkler, M (Vinkler, Michal)

Abstract: Avian egg white is essential for protecting and nourishing bird embryos during their development. Being produced in the female magnum, variability in hen oviduct gene expression may affect egg white composition in domestic chickens. Since traditional poultry breeds may represent a source of variation, in the present study we describe the egg white proteome (mass spectrometry) and corresponding magnum transcriptome (high-throughput sequencing) for 20 hens from five domestic fowl breeds (large breeds: Araucana, Czech golden pencilled, Minorca; and small breeds: Booted bantam, Rosecomb bantam). In total, we identified 189 egg white proteins and 16391 magnum-expressed genes. The majority of egg white protein content comprised proteins with an antimicrobial function. Despite general similarity, Between-class Principal Component Analysis revealed significant breed-specific variability in protein abundances, differentiating especially small and large breeds. Though we found strong association between magnum mRNA expression and egg white protein abundance across genes, coinertia analysis revealed no transcriptome/proteome costructure at the individual level. Our study is the first to show variation in protein abundances in egg white across chicken breeds with potential effects on egg quality, biosafety, and chick development. The observed interindividual variation probably results from post-transcriptional regulation creating a discrepancy between proteomic and transcriptomic data.

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Record 20 of 214
Title: Covalent Functionalization of Exfoliated Arsenic with Chlorocarbene

Author(s): Sturala, J (Sturala, Jiri); Ambrosi, A (Ambrosi, Adriano); Sofer, Z (Sofer, Zdenek); Pumera, M (Pumera, Martin)

Abstract: Few-layer and monolayer arsenic (arsenene) materials have been attracting great attention mainly from a theoretical perspective. Chemical modification of these materials would expand significantly the range of their applications. Here, we describe a chlorocarbene-mediated modification of exfoliated layered arsenic materials. Carbene-based species are highly reactive and offer further possibilities of functionalization. Our approach for modifying the arsenic surface by chlorocarbene generated from organolithium and dichloromethane resulted in a large surface coverage and a highly luminescent functionalized material, opening the door for its application in modern optoelectronic devices.

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Record 21 of 214
Title: Structural and physical characterization of NpPt2In7

Author(s): Klimczuk, T (Klimczuk, T.); Shick, AB (Shick, A. B.); Khmelevskyi, S (Khmelevskyi, S.); Kozub, AL (Kozub, A. L.); Kolincio, KK (Kolincio, K. K.); Griveau, JC (Griveau, J. -C.); Colineau, E (Colineau, E.); Eloirdi, R (Eloirdi, R.); Caciuffo, R (Caciuffo, R.)

Abstract: A new neptunium intermetallic compound, NpPt2In7, has been synthesized in polycrystalline form and characterized by several macroscopic techniques. A Rietveld analysis of its powder X-ray diffraction pattern shows that NpPt2In7 crystallizes in a tetragonal lattice with I4/mmm symmetry and lattice parameters alpha = 4.58471(3) angstrom, c = 21.5065(3) angstrom. Magnetic susceptibility, electrical resistivity, Hall effect, and heat capacity measurements indicate a metallic character and the occurrence of antiferromagnetic order below a Neel temperature T-N = 23 K. The transition is exceptionally robust and T-N decreases by 0.2 K under a magnetic field of 9 T. A modified Curie-Weiss fit of the high-temperature magnetic susceptibility curve chi(T) gives an effective magnetic moment mu(eff) = 2.54 mu(B) close to the value expected for trivalent Np. Low temperature heat capacity measurements give a reduced Sommerfeld linear coefficient close to 25 mJ mol(-1)K(-2) and a Debye Temperature Theta(D) = 181 K. First principles, correlated-band electronic structure calculations suggest that the neptunium magnetic moment in NpPt2In7 is localized and that a quasi-two-dimensional antiferromagnetic structure could result from the competition of very weak interlayer interactions leading to very anisotropic properties. (C) 2018 Elsevier B.V. All rights reserved.

Author Identifiers:

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Record 22 of 214

Title: Selectivity for La3+ ion by synthesized 4-((5-methylfuran-2-yl) methylene)hydrazono)methyl)phenol receptor and its spectral analysis

Author(s): Mohan, B (Mohan, Brij); Modi, K (Modi, Krunal); Patel, C (Patel, Chirag); Bhatia, P (Bhatia, Pankaj); Kumar, P (Kumar, Parveen); Kumar, A (Kumar, Ashwani); Sharma, HK (Sharma, Harish Kumar)

Abstract: The functionalized molecules with specific molecular sites appear to be a promising approach for detection of cation in UV-visible and fluorescence spectroscopy. The synthesized receptor 4-((5-methylfuran-2-yl)methylene) hydrazono)methyl)phenol MFMHMP was found selective for La3+ among Ag+, K+, Na+, Be2+, Mg2+, Ca2+, Eu3+, Al3+, La3+, Zr4+, Th4+, UO22+, Fe3+, Fe2+, Co3+, Ni2+, Cu2+, Zn2+, Cd2+ and Hg2+ metal ions used as their nitrates by UV-visible spectroscopy and fluorescence spectroscopy. The binding nature of MFMHMP with La3+ ion was analyzed by UV-visible, fluorescence, IR, mass spectroscopy and cyclic voltammetric studies. The stoichiometry was established to be 1:1 by Benesi-Hildebrand, mole-ratio method and method of continuous variation (Job's method) with good association affinity K = 6245 x 10(4)M(-1). Computational studies and Density functional theory (DFT) calculation gives the proof of electron transfer during excitation and emission. Binding energy of complex through Density Function Theory -62.387 kcal/mol has also indication of strong binding. The electron transfer energy of Higher occupied molecular orbital (HOMO) to Lower unoccupied molecular orbital (LUMO) is about 4.662 eV for MFMHMP+La3+ Complex. Among that all transitions HOMO -> LUMO + 8 and HOMO -> LUMO + 9 play a key role for the blue shift transition during complexation. (C) 2018 Elsevier B.V. All rights reserved.

Accession Number: WOS:000442063000073

PubMed ID: 29980059

Record 23 of 214

Title: Magnetic Diversity in Heteroisocorroles: Aromatic Pathways in 10-Heteroatom-Substituted Isocorroles

Author(s): Foroutan-Nejad, C (Foroutan-Nejad, Cina); Ghosh, A (Ghosh, Abhik)

Abstract: A recent study on magnetically induced currents in 10-isocorrole derivatives indicated that both the free-base and metal-complexed forms of the unsubstituted macro-cycle are homoaromatic. Furthermore, depending on the substituents at the 10-position, the aromatic character was found to swing between substantially homoaromatic to substantially antihomoaromatic. Heteroisocorroles, in which the saturated 10-position has been replaced by a heteroatom-containing group X, are predicted to exhibit even more dramatic variations in aromatic character, ranging from strongly aromatic (X = O, NH, PH, and S) to strongly antiaromatic (X = BH and CO). Interestingly, the experimentally studied X = SiMe2 case does not appear to sustain a significant global ring current.

Accession Number: WOS:000451992500140

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Author	ResearcherID Number	ORCID Number
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Record 24 of 214

Title: Moving to the Edge-Cloud-of-Things: Recent Advances and Future Research Directions

Author(s): Bangui, H (Bangui, Hind); Rakrak, S (Rakrak, Said); Raghay, S (Raghay, Said); Buhnova, B (Buhnova, Barbora)

Abstract: Cloud computing has significantly enhanced the growth of the Internet of Things (IoT) by ensuring and supporting the Quality of Service (QoS) of IoT applications. However, cloud services are still far from IoT devices. Notably, the transmission of IoT data experiences network issues, such as high latency. In this case, the cloud platforms cannot satisfy the IoT applications that require real-time response. Yet, the location of cloud services is one of the challenges encountered in the evolution of the IoT paradigm. Recently, edge cloud computing has been proposed to bring cloud services closer to the IoT end-users, becoming a promising paradigm whose pitfalls and challenges are not yet well understood. This paper aims at presenting the leading-edge computing concerning the movement of services from centralized cloud platforms to decentralized platforms, and examines the issues and challenges introduced by these highly distributed environments, to support engineers and researchers who might benefit from this transition.

Accession Number: WOS:000451527400042

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Record 25 of 214

Title: Intraoperative Thermography of the Electrical Stimulation Mapping: A Safety Control Study

Author(s): Janca, R (Janca, R.); Jezdik, P (Jezdik, P.); Jahodova, A (Jahodova, A.); Kudr, M (Kudr, M.); Benova, B (Benova, B.); Celakovsky, P (Celakovsky, P.); Zamecnik, J (Zamecnik, J.); Komarek, V (Komarek, V.); Liby, P (Liby, P.); Tichy, M (Tichy, M.); Krsek, P (Krsek, P.)

Abstract: A standard procedure for continuous intra-operative monitoring of the integrity of the corticospinal tracts by eliciting muscle responses is the electric stimulation mapping (ESM). However, standard ESM protocols are ineffective in 20% of young children. We have developed a novel, highly efficient paradigm consisting of short-time burst (30 ms) of high frequency (500 Hz) and high peak current (<= 100 mA), which may cause local tissue overheating. The presented safety control study was therefore designed. The infrared thermography camera captured to-be-resected cortex of 13 patients in vivo during ESM. Thermograms were image processed to reveal discrete ESM thermal effect of currents from 10 to 100 mA. Peak 100 mA currents induced a maximal increase in temperature of 3.1 degrees C, 1.23 +/- 0.72 degrees C in average. The warming correlated with stimulating electrode resistance (p < 0.001). The measurement uncertainty was estimated +/- 1.01 degrees C for the most skeptical conditions. The histopathological evaluation of stimulated tissue (performed in all cases) did not show any destructive changes. Our study demonstrates the ability of the thermographic camera to measure the discrete thermal effect of the ESM. The results provide evidence for the safety of the proposed protocol for full range currents with minimal risk of brain tissue damage.

Accession Number: WOS:000451250400005

PubMed ID: 30475703

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Record 26 of 214

Title: Hybridization-facilitated genome merger and repeated chromosome fusion after 8 million years

Author(s): Mandakova, T (Mandakova, Terezie); Guo, XY (Guo, Xinyi); Ozudogru, B (Ozudogru, Baris); Mummenhoff, K (Mummenhoff, Klaus); Lysak, MA (Lysak, Martin A.)

Abstract: The small genus Ricotia (nine species, Brassicaceae) is confined to the eastern Mediterranean. By comparative chromosome painting and a dated multi-gene chloroplast phylogeny, we reconstructed the origin and subsequent evolution of Ricotia. The ancestral Ricotia genome originated through hybridization between two older genomes with n = 7 and n = 8 chromosomes, respectively, on the Turkish mainland during the Early Miocene (c. 17.8 million years ago, Ma). Since then, the allotetraploid (n = 15) genome has been altered by two independent descending dysploidies (DD) to n = 14 in Ricotia aucheri and the Tenuifolia clade (2 spp.). By the Late Miocene (c. 10 Ma), the latter clade started to evolve in the most diverse Ricotia core clade (6 spp.), the process preceded by a DD event to n = 13. It is noteworthy that this dysploidy was mediated by a unique chromosomal rearrangement, merging together the same two chromosomes as were merged during the origin of a fusion chromosome within the paternal n = 7 genome c. 20 Ma. This shows that within a time period of c. 8 Myr genome evolution can repeat itself and that structurally very similar chromosomes may originate repeatedly from the same ancestral chromosomes by different

pathways (end-to-end translocation versus nested chromosome insertion).
Accession Number: WOS:000449986700005
PubMed ID: 30101476
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ISSN: 0960-7412
eISSN: 1365-313X

Record 27 of 214
Title: Adsorption of 17 alpha-ethynyl estradiol and beta-estradiol on graphene oxide surface: An experimental and computational study
Author(s): Borthakur, P (Borthakur, Priyakshree); Boruah, PK (Boruah, Puma K.); Das, MR (Das, Manash R.); Kulik, N (Kulik, Natallia); Minofar, B (Minofar, Babak)
Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 269 **Pages:** 160-168 **DOI:** 10.1016/j.molliq.2018.08.013 **Published:** NOV 1 2018
Abstract: Adsorption of endocrine disrupting chemicals (EDCs) such as 17 alpha-ethynyl estradiol and beta-estradiol on sp(2) hybridized graphene oxide (GO) sheets as an efficient adsorbent was carried out. The effect of different experimental parameters such as the concentration of adsorbent and adsorbate as well as pH of the medium were investigated. It was observed that both 17 alpha-ethynyl estradiol and beta-estradiol molecules interact with the aromatic skeleton of graphene oxide ring by hydrogen bonding and electrostatic interactions between the oxygen containing functional groups of GO and -OH groups of micropollutant molecules in addition to pi-pi interactions between the pi-electrons of graphene oxide and the aromatic rings of the micropollutant molecules. It was found that the adsorption was facilitated in acidic medium and maximum adsorption efficiency of GO was found to be 98.46% and 97.19% for 17 alpha-ethynyl estradiol and beta-estradiol, respectively at pH 3 within 50 min. Classical molecular dynamics (MD) simulations were performed to analyze the adsorption process in the molecular level to support the experimental findings. The results obtained from the computational study show good agreement with the experimental findings. (C) 2018 Published by Elsevier B.V.
Accession Number: WOS:000447482500018
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ISSN: 0167-7322
eISSN: 1873-3166

Record 28 of 214
Title: Resolving the rapid plant radiation of early diverging lineages in the tropical Zingiberales: Pushing the limits of genomic data
Author(s): Carlsen, MM (Carlsen, Monica M.); Fer, T (Fer, Tomas); Schmickl, R (Schmickl, Roswitha); Leong-Skornickova, J (Leong-Skornickova, Jana); Newman, M (Newman, Mark); Kress, WJ (Kress, W. John)
Source: MOLECULAR PHYLOGENETICS AND EVOLUTION **Volume:** 128 **Pages:** 55-68 **DOI:** 10.1016/j.ympev.2018.07.020 **Published:** NOV 2018
Abstract: Many cases of rapid evolutionary radiations in plant and animal lineages are known; however phylogenetic relationships among these lineages have been difficult to resolve by systematists. Increasing amounts of genomic data have been sequentially applied in an attempt to resolve these radiations, dissecting their evolutionary patterns into a series of bifurcating events. Here we explore one such rapid radiation in the tropical plant order Zingiberales (the bananas and relatives) which includes eight families, approximately 110 genera, and more than 2600 species. One Glade, the "Ginger families", including (Costaceae + Zingiberaceae) (Marantaceae + Cannaceae), has been well-resolved and well-supported in all previous studies. However, well-supported reconstructions among the "Banana families" (Musaceae, Heliconiaceae, Lowiaceae, Strelitziaceae), which most likely diverged about 90 Mya, have been difficult to confirm. Supported with anatomical, morphological, single locus, and genome-wide data, nearly every possible phylogenetic placement has been proposed for these families. In an attempt to resolve this complex evolutionary event, hybridization-based target enrichment was used to obtain sequences from up to 378 putatively orthologous low-copy nuclear genes (all 960 bp). Individual gene trees recovered multiple topologies among the early divergent lineages, with varying levels of support for these relationships. One topology of the "Banana families" (Musaceae (Heliconiaceae (Lowiaceae + Strelitziaceae))), which has not been suggested until now, was almost consistently recovered in all multilocus analyses of the nuclear dataset (concatenated - ExaML, coalescent - ASTRAL and ASTRID, supertree - MRL, and Bayesian concordance - BUCKy). Nevertheless, the multiple topologies recovered among these lineages suggest that even large amounts of genomic data might not be able to fully resolve relationships at this phylogenetic depth. This lack of well-supported resolution could suggest methodological problems (i.e., violation of model assumptions in both concatenated and coalescent analyses) or more likely reflect an evolutionary history shaped by an explosive, rapid, and nearly simultaneous polychotomous radiation in this group of plants towards the end of the Cretaceous, perhaps driven by vertebrate pollinator selection.
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PubMed ID: 30063997
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Record 29 of 214
Title: Molecular and Morphological Diversity of the Oxymonad Genera Monocercomonoides and Blattamonas gen. nov.
Author(s): Treitli, SC (Treitli, Sebastian C.); Kotyk, M (Kotyk, Michael); Yubuki, N (Yubuki, Naoji); Jirounkova, E (Jirounkova, Eliska); Vlasakova, J (Vlasakova, Jitka); Smejkalova, P (Smejkalova, Pavla); Sipek, P (Sipek, Petr); Cepicka, I (Cepicka, Ivan); Hampl, V (Hampl, Vladimir)
Source: PROTIST **Volume:** 169 **Issue:** 5 **Pages:** 744-783 **DOI:** 10.1016/j.protis.2018.06.005 **Published:** NOV 2018
Abstract: Oxymonads are a group of flagellates living as gut symbionts of insects or vertebrates. They have several unique features, one of them being the absence of mitochondria. Diversity of this group is seriously understudied, which is particularly true for small species from the family Polymastigidae. We isolated 34 strains of oxymonads with Polymastigidae-like morphology from 24 host species and unused cesspits and sequenced the SSU rRNA gene. Our strains formed two clades in the phylogenetic tree with Streblomastix strix branching between them. This topology was also supported by a three-gene phylogenetic analysis. Despite considerable genetic differences between the clades, light and electron microscopy revealed only subtle differences. The larger Glade is considered genus Monocercomonoides and the isolates belonging here were classified into three new species (including the first potentially free-living species), two previously described species, and three unclassified lineages. The smaller Glade, here described as Blattamonas gen. nov., consists of three newly described species. Concomitantly with the description of Blattamonas, we elevate the Monocercomonoides subgenus Brachymonas to the genus level. Our study shows that, despite their conserved morphology, the molecular diversity of Polymastigidae-like oxymonads is broad and represents a substantial part of the diversity of oxymonads. (C) 2018 Elsevier GmbH. All rights reserved.
Accession Number: WOS:000444618900009
PubMed ID: 30138782
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ISSN: 1434-4610

Record 30 of 214
Title: Extremely rapid isotropic irradiation of nanoparticles with ions generated in situ by a nuclear reaction
Author(s): Havlik, J (Havlik, Jan); Petrakova, V (Petrakova, Vladimira); Kucka, J (Kucka, Jan); Raabova, H (Raabova, Helena); Panek, D (Panek, Dalibor); Stepan, V (Stepan, Vaclav); Cilova, ZZ (Cilova, Zuzana Zlamalova); Reineck, P (Reineck, Philipp); Stursa, J (Stursa, Jan); Kucera, J (Kucera, Jan); Hruby, M (Hruby, Martin); Cigler, P (Cigler, Petr)
Source: NATURE COMMUNICATIONS **Volume:** 9 **Article Number:** 4467 **DOI:** 10.1038/s41467-018-06789-8 **Published:** OCT 26 2018
Abstract: Energetic ions represent an important tool for the creation of controlled structural defects in solid nanomaterials. However, the current preparative irradiation techniques in accelerators show significant limitations in scaling-up, because only very thin layers of nanoparticles can be efficiently and homogeneously irradiated. Here, we show an easily scalable method for rapid irradiation of nanomaterials by light ions formed homogeneously in situ by a nuclear reaction. The target nanoparticles are embedded in B_2O_3 and placed in a neutron flux. Neutrons captured by B-10 generate an isotropic flux of energetic a particles and Li-7(+) ions that uniformly irradiates the surrounding nanoparticles. We produced 70 g of fluorescent nanodiamonds in an approximately 30-minute irradiation session, as well as fluorescent silicon carbide nanoparticles. Our method thus increased current preparative yields by a factor of 10(2)-10(3). We envision that our technique will increase the production of ion-irradiated nanoparticles, facilitating their use in various applications.
Accession Number: WOS:000448414100017
PubMed ID: 30367036

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Hruby, Martin	H-6479-2014	

Record 31 of 214

Title: Overcoming Volume Selectivity of Dipolar Recoupling in Biological Solid-State NMR Spectroscopy

Author(s): Tosner, Z (Tosner, Zdenek); Sarkar, R (Sarkar, Riddhiman); Becker-Baldus, J (Becker-Baldus, Johanna); Glaubitz, C (Glaubitz, Clemens); Wegner, S (Wegner, Sebastian); Engelke, F (Engelke, Frank); Glaser, SJ (Glaser, Steffen J.); Reif, B (Reif, Bernd)

Abstract: Dipolar recoupling in solid-state NMR is an essential method for establishing correlations between nuclei that are close in space. In applications on protein samples, the traditional experiments like ramped and adiabatic DCP suffer from the fact that dipolar recoupling occurs only within a limited volume of the sample. This selection is dictated by the radiofrequency (rf) field inhomogeneity profile of the excitation solenoidal coil. We employ optimal control strategies to design dipolar recoupling sequences with substantially larger responsive volume and increased sensitivity. We show that it is essential to compensate for additional temporal modulations induced by sample rotation in a spatially inhomogeneous rf field. Such modulations interfere with the pulse sequence and decrease its performance. Using large-scale optimizations we developed pulse schemes for magnetization transfer from amide nitrogen to carbonyl (NCO) as well as aliphatic carbons (NCA). Our experiments yield a signal intensity increased by a factor of 1.5 and 2.0 for NCA and NCO transfers, respectively, compared to conventional ramped DCP sequences. Consistent results were obtained using several biological samples and NMR instruments.

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Record 32 of 214

Title: Spin-disorder resistivity of random fcc-NiFe alloys

Author(s): Drcha, V (Drcha, V); Kudrnovsky, J (Kudrnovsky, J.); Wagenknecht, D (Wagenknecht, D.); Turek, I (Turek, I)

Abstract: The spin-disorder resistivity (SDR) of a disordered fcc-(Ni1-x, Fe-x) alloy is determined from first principles. We identify the SDR at and above the critical temperature with the residual resistivity of the corresponding paramagnetic state evaluated in the framework of the disordered local moment (DLM) model. The underlying electronic structure is determined by means of the tight-binding linear muffin-tin orbital method, which employs the coherent potential approximation (CPA) to describe both the DLM state and the chemical disorder in alloys. An extension of the DLM fixed-spin moment method for two independent magnetic moments is used and combined with the paramagnetic lattice gas entropy to determine local moments by minimizing the corresponding free energy. The effect of phonon scattering is included through the mapping of static atomic displacements into a multicomponent random alloy which is then treated in the CPA. Finally, the Kubo-Greenwood-CPA approach is employed to estimate the SDR. We also address the problem of the validity of the Matthiessen rule at the Curie point. Good agreement of calculated and measured SDR is obtained over the whole studied concentration range; the results point to the importance of nonzero Ni magnetic moments in the limit of pure nickel.

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

Record 33 of 214

Title: Disentangling direct and indirect effects of water availability, vegetation, and topography on avian diversity

Author(s): Remes, V (Remes, Vladimir); Harmackova, L (Harmackova, Lenka)

Abstract: Climate is a major driver of species diversity. However, its effect can be either direct due to species physiological tolerances or indirect, whereby wetter climates facilitate more complex vegetation and consequently higher diversity due to greater resource availability. Yet, studies quantifying both direct and indirect effects of climate on multiple dimensions of diversity are rare. We used extensive data on species distributions, morphological and ecological traits, and vegetation across Australia to quantify both direct (water availability) and indirect (habitat diversity and canopy height) effects of climate on the species richness (SR), phylogenetic diversity (PD), and functional diversity (FD) of 536 species of birds. Path analyses revealed that SR increased with wetter climates through both direct and indirect effects, lending support for the influence of both physiological tolerance and vegetation complexity. However, residual PD and residual FD (adjusted for SR by null models) were poorly predicted by environmental conditions. Thus, the FD and PD of Australian birds mostly evolved in concert with SR, with the possible exception of the higher-than-expected accumulation of avian lineages in wetter and more productive areas in northern and eastern Australia (with high residual PD), permitted probably by older biome age.

Record 34 of 214

Title: Computed stabilization for a giant fullerene endohedral: Y2C2@C-1(1660)-C-108

Author(s): Slanina, Z (Slanina, Zdenek); Uhlik, F (Uhlik, Filip); Pan, CW (Pan, Changwang); Akasaka, T (Akasaka, Takeshi); Lu, X (Lu, Xing); Adamowicz, L (Adamowicz, Ludwik)

Abstract: The very recently prepared clusterfullerene Y2C2@C-1(1660)-C-108 is computed and the observed structural features are confirmed, including the quasi-linear arrangement of the encapsulate and its near-triple CC bond. Its stability is explained by sizeable encapsulation energy. The endohedral stability is evaluated at both DFT and MP2 levels.

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Author	ResearcherID Number	ORCID Number
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Record 35 of 214

Title: CAVER Analyst 2.0: analysis and visualization of channels and tunnels in protein structures and molecular dynamics trajectories

Author(s): Jurcik, A (Jurcik, Adam); Bednar, D (Bednar, David); Byska, J (Byska, Jan); Marques, SM (Marques, Sergio M.); Furmanova, K (Furmanova, Katarina); Daniel, L (Daniel, Lukas); Kokkonen, P (Kokkonen, Piia); Brezovsky, J (Brezovsky, Jan); Strnad, O (Strnad, Ondrej); Stourac, J (Stourac, Jan); Pavelka, A (Pavelka, Antonin); Manak, M (Manak, Martin); Damborsky, J (Damborsky, Jiri); Kozlikova, B (Kozlikova, Barbora)

Abstract: Motivation: Studying the transport paths of ligands, solvents, or ions in transmembrane proteins and proteins with buried binding sites is fundamental to the understanding of their biological function. A detailed analysis of the structural features influencing the transport paths is also important for engineering proteins for biomedical and biotechnological applications.

Results: CAVER Analyst 2.0 is a software tool for quantitative analysis and real-time visualization of tunnels and channels in static and dynamic structures. This version provides the users with many new functions, including advanced techniques for intuitive visual inspection of the spatiotemporal behavior of tunnels and channels. Novel integrated algorithms allow an efficient analysis and data reduction in large protein structures and molecular dynamic simulations.

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PubMed ID: 29741570

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ISSN: 1367-4803

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Record 36 of 214

Title: Buckyball Difluoride F-2(-)@C-60(+)-A Single-Molecule Crystal

Author(s): Foroutan-Nejad, C (Foroutan-Nejad, Cina); Straka, M (Straka, Michal); Fernandez, I (Fernandez, Israel); Frenking, G (Frenking, Gernot)

Source: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 57 **Issue:** 42 **Pages:** 13931-13934 **DOI:** 10.1002/anie.201809699 **Published:** OCT 15 2018

Abstract: We report the F-2@C-60 system as the first example of an endohedral fullerene in which C-60 acts as a cation C-60(+) interacting with endohedral anion, F-2(-). Our state-of-the-art computations reveal that in F-2@C-60, despite of the known high electron affinity of C-60, an electron is transferred from C-60 to F-2 resulting in the F-2(-)@C-60(+) system. The F-F bond length in F-2@C-60 is substantially longer than in free F-2, which is the result of electron-transfer to the antibonding sigma(u) molecular orbital of F-2. Interestingly, although there is a full charge-transfer of one electron between C-60 and F-2, only negligible delocalized covalent interactions are found between F-2(-) and C-60(+) which is a reminiscent of ionic crystals. Therefore, F-2(-)@C-60(+) can be considered as a single-molecule crystal. The other encapsulated halogens in C-60 do not show such behavior.

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PubMed ID: 30152567

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DONOSTIA INTERNATIONAL PHYSICS CTR., DIPC	C-3171-2014	
Straka, Michal		0000-0002-7857-4990

ISSN: 1433-7851

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Record 37 of 214

Title: Modeling of solid-liquid interfaces using scaled charges: rutile (110) surfaces

Author(s): Biriukov, D (Biriukov, Denys); Kroutil, O (Kroutil, Ondrej); Predota, M (Predota, Milan)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 20 **Issue:** 37 **Pages:** 23954-23966 **DOI:** 10.1039/c8cp04535f **Published:** OCT 7 2018

Abstract: Electronic continuum correction (ECC) has been proven to bring significant improvement in the modeling of interactions of ions (especially multivalent) in aqueous solutions. We present a generalization and the first application of this approach to modeling solid-liquid interfaces, which are omnipresent in physical chemistry, geochemistry, and biophysics. Scaling charges of the top layer of surface atoms makes the existing solid models compatible with the ECC models of ions and molecules, allowing the use of modified force fields for a more accurate investigation of interactions of various metal and metal-oxide surfaces with aqueous solutions, including complex biomolecules and multivalent ions. We have reparametrized rutile (110) models with different surface charge densities (from 0 to -0.416 C m(-2)) and adopted/developed scaled charge force fields for ions, namely Na+, Rb+, Sr2+, and Cl-. A good agreement of the obtained molecular dynamics (MD) data with X-ray experiments and previously reported MD results was observed, but changes in the occupancy of various adsorption sites were observed and discussed in detail.

Accession Number: WOS:000446766300012

PubMed ID: 30209469

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Record 38 of 214

Title: Molecular and Cytogenetic Study of East African Highland Banana

Author(s): Nemeckova, A (Nemeckova, Alzbeta); Christelova, P (Christelova, Pavla); Cizkova, J (Cizkova, Jana); Nyine, M (Nyine, Moses); Van den Houwe, I (Van den Houwe, Ines); Svacina, R (Svacina, Radim); Uwimana, B (Uwimana, Brigitte); Swennen, R (Swennen, Rony); Dolezel, J (Dolezel, Jaroslav); Hribova, E (Hribova, Eva)

Source: FRONTIERS IN PLANT SCIENCE **Volume:** 9 **Article Number:** 1371 **DOI:** 10.3389/fpls.2018.01371 **Published:** OCT 4 2018

Abstract: East African highland bananas (EAHBs) are staple food crop in Uganda, Tanzania, Burundi, and other countries in the African Great Lakes region. Even though several morphologically different types exist, all EAHBs are triploid and display minimal genetic variation. To provide more insights into the genetic variation within EAHBs, genotyping using simple sequence repeat (SSR) markers, molecular analysis of ITS1-5.8S-ITS2 region of ribosomal DNA locus, and the analysis of chromosomal distribution of ribosomal DNA sequences were done. A total of 38 triploid EAHB accessions available in the Musa germplasm collection (International Transit Centre, Leuven, Belgium) were characterized. Six diploid accessions of Musa acuminata ssp. zebrina, ssp. banksii, and ssp. malaccensis representing putative parents of EAHBs were included in the study. Flow cytometric estimation of 2C nuclear DNA content revealed small differences (max similar to 6.5%) in genome size among the EAHB clones. While no differences in the number of 45S and 5S rDNA loci were found, genotyping using 19 SSR markers resulted in grouping the EAHB accessions into four clusters. The DNA sequence analysis of the internal transcribed spacer region indicated a relation of EAHB clones with M. acuminata and, surprisingly, also with M. schizocarpa. The results suggest that EAHB cultivars originated from a single hybrid clone with M. acuminata ssp. zebrina and ssp. banksii being its most probable parents. However, M. schizocarpa seems to have contributed to the formation of this group of banana.

Accession Number: WOS:000446330600001

PubMed ID: 30337933

ISSN: 1664-462X

Record 39 of 214

Title: Host specificity driving genetic structure and diversity in ectoparasite populations: Coevolutionary patterns in Apodemus mice and their lice

Author(s): Martinu, J (Martinu, Jana); Hypsa, V (Hypsa, Vaclav); Stefka, J (Stefka, Jan)

Source: ECOLOGY AND EVOLUTION **Volume:** 8 **Issue:** 20 **Pages:** 10008-10022 **DOI:** 10.1002/ece3.4424 **Published:** OCT 2018

Abstract: A degree of host specificity, manifested by the processes of host-parasite cospeciations and host switches, is assumed to be a major determinant of parasites' evolution. To understand these patterns and formulate appropriate ecological hypotheses, we need better insight into the coevolutionary processes at the intraspecific level, including the maintenance of genetic diversity and population structure of parasites and their hosts. Here, we address these questions by analyzing large-scale molecular data on the louse Polyplax serrata and its hosts, mice of the genus Apodemus, across a broad range of European localities. Using mitochondrial DNA sequences and microsatellite data, we demonstrate the general genetic correspondence of the Apodemus/Polyplax system to the scenario of the postglacial recolonization of Europe, but we also show several striking discrepancies. Among the most interesting are the evolution of different degrees of host specificity in closely related louse lineages in sympatry, or decoupled population structures of the host and parasites in central Europe. We also find strong support for the prediction that parasites with narrower host specificity possess a lower level of genetic diversity and a deeper pattern of interpopulation structure as a result of limited dispersal and smaller effective population size.

Accession Number: WOS:000449529800005

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ISSN: 2045-7758

Record 40 of 214

Title: Complete genome sequences of two strains of Treponema pallidum subsp pertenue from Indonesia: Modular structure of several treponemal genes

Author(s): Strouhal, M (Strouhal, Michel); Mikalova, L (Mikalova, Lenka); Haviernik, J (Haviernik, Jan); Knauf, S (Knauf, Sascha); Bruisten, S (Bruisten, Sylvia); Noordhoek, GT (Noordhoek, Gerda T.); Oppelt, J (Oppelt, Jan); Cejkova, D (Cejkova, Darina); Smajs, D (Smajs, David)

Abstract: Background

Treponema pallidum subsp. pertenue (TPE) is the causative agent of yaws, a multistage disease endemic in tropical regions in Africa, Asia, Oceania, and South America. To date, seven TPE strains have been completely sequenced and analyzed including five TPE strains of human origin (CDC-2, CDC 2575, Gauthier, Ghana-051, and Samoa D) and two TPE strains isolated from the baboons (Fribourg-Blanc and LMNP-1). This study revealed the complete genome sequences of two TPE strains, Kampung Dalan K363 and Sei Geringging K403, isolated in 1990 from villages in the Pariaman region of Sumatra, Indonesia and compared these genome sequences with other known TPE genomes.

Methodology/principal findings

The genomes were determined using the pooled segment genome sequencing method combined with the Illumina sequencing platform resulting in an average coverage depth of 1,021x and 644x for the TPE Kampung Dalan K363 and TPE Sei Geringging K403 genomes, respectively. Both Indonesian TPE strains were genetically related to each other and were more distantly related to other, previously characterized TPE strains. The modular character of several genes, including TP0136 and TP0858 gene orthologs, was identified by analysis of the corresponding sequences. To systematically detect genes potentially having a modular genetic structure, we performed a whole genome analysis-of-occurrence of direct or inverted repeats of 17 or more nucleotides in length. Besides in tpr genes, a frequent presence of repeats was found in the genetic regions spanning TP0126-TP0136, TP0856-TP0858, and TP0896 genes.

Conclusions/significance

Comparisons of genome sequences of TPE Kampung Dalan K363 and Sei Geringging K403 with other TPE strains revealed a modular structure of several genomic loci including the TP0136, TP0856, and TP0858 genes. Diversification of TPE genomes appears to be facilitated by intra-strain genome recombination events.

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ISSN: 1935-2735

Record 41 of 214

Title: Fecal microbiota associated with phytohaemagglutinin-induced immune response in nestlings of a passerine bird

Author(s): Kreisinger, J (Kreisinger, Jakub); Schmiedova, L (Schmiedova, Lucie); Petrzelkova, A (Petrzelkova, Adela); Tomasek, O (Tomasek, Oldrich); Adamkova, M (Adamkova, Marie); Michalkova, R (Michalkova, Romana); Martin, JF (Martin, Jean-Francois); Albrecht, T (Albrecht, Tomas)

Abstract: The vertebrate gastrointestinal tract is inhabited by a diverse community of bacteria, the so-called gut microbiota (GM). Research on captive mammalian models has revealed tight mutual interactions between immune functions and GM. However, our knowledge of GM versus immune system interactions in wild populations and nonmammalian species remains poor. Here, we focus on the association between GM community structure and immune response measured via the phytohaemagglutinin (PHA) skin swelling test in 12-day-old nestlings of a passerine bird, the barn swallow (Hirundo rustica). The PHA test, a widely used method in field ecoimmunology, assesses cell-mediated immunity. GM structure was inferred based on high-throughput 16S rRNA sequencing of microbial communities in fecal samples. We did not find any association between PHA response and GM diversity; however, our data revealed that the intensity of PHA response was correlated with differences in GM composition at the whole-community level. Ten bacterial operational taxonomic units corresponding to both putative commensal and pathogens were identified as drivers of the compositional variation. In conclusion, our study suggests existence of GM versus immune system interactions in a free-living nonmammalian species, which corresponds with previous research on captive vertebrates.

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Record 42 of 214

Title: Activation Process of ONU in EPON/GPON/XG-PON/NG-PON2 Networks

Author(s): Horvath, T (Horvath, Tomas); Munster, P (Munster, Petr); Oujersky, V (Oujersky, Vaclav); Vojtech, J (Vojtech, Josef)

Abstract: This article presents a numerical implementation of the activation process for gigabit and 10 gigabit next generation and Ethernet passive optical networks. The specifications are completely different because GPON, XG-PON and NG-PON2 were developed by the International Telecommunication Union, whereas Ethernet PON was developed by the Institute of Electrical and Electronics Engineers. The speed of an activation process is the most important in a blackout scenario because end optical units have a timer after expiration transmission parameters are discarded. Proper implementation of an activation process is crucial for eliminating inadvisable delay. An OLT chassis is dedicated to several GPON (or other standard) cards. Each card has up to eight or 16 GPON ports. Furthermore, one GPON port can operate with up to 64/128 ONUs. Our results indicate a shorter duration activation process (due to a shorter frame duration) in Ethernet-based PON, but the maximum split ratio is only 1:32 instead of up to 1:64/128 for gigabit PON and newer standards. An optimization improves the reduction time for the GPON activation process with current PLOAM messages and with no changes in the transmission convergence layer. We reduced the activation time from 215 ms to 145 ms for 64 ONUs.

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ISSN: 2076-3417

Record 43 of 214

Title: Structural Dynamics of Lateral and Diagonal Loops of Human Telomeric G-Quadruplexes in Extended MD Simulations

Author(s): Islam, B (Islam, Barira); Stadlbauer, P (Stadlbauer, Petr); Krepl, M (Krepl, Miroslav); Havrila, M (Havrila, Marek); Haider, S (Haider, Shozeb); Sponer, J (Sponer, Jiri)

Abstract: The NMR solution structures of human telomeric (Htel) G-quadruplexes (GQs) are characterized by the presence of two lateral loops complemented by either diagonal or propeller loops. Bases of a given loop can establish interactions within the loop as well as with other loops and the flanking bases. This can lead to a formation of base alignments above and below the GQ stems. These base alignments are known to affect the loop structures and relative stabilities of different Htel GQ folds. We have carried out a total of 217 mu s of classical (unbiased) molecular dynamics (MD) simulations starting from the available solution structures of Htel GQs to characterize structural dynamics of the lateral and diagonal loops, using several recent AMBER DNA force-field variants. As the loops are involved in diverse stacking and H-bonding interactions, their dynamics is slow, and extended sampling is required to capture different conformations. Nevertheless, although the simulations are far from being quantitatively converged, the data suggest that multiple 10 Hs-scale simulations can provide a quite good assessment of the loop conformational space as described by the force field. The simulations indicate that the lateral loops may sample multiple

coexisting conformations, which should be considered when comparing simulations with the NMR models as the latter include ensemble averaging. The adenine-thymine Watson-Crick arrangement was the most stable base pairing in the simulations. Adenine adenine and thymine-thymine base pairs were also sampled but were less stable. The data suggest that the description of lateral and diagonal GQ loops in contemporary MD simulations is considerably more realistic than the description of propeller loops, though definitely not flawless.

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PubMed ID: 30183284

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Record 44 of 214

Title: Dosimetry as a Catch in Radiobiology Experiments

Author(s): Sefl, M (Sefl, Martin); Brabcova, KP (Brabcova, Katerina Pachnerova); Stepan, V (Stepan, Vaclav)

Source: RADIATION RESEARCH   **Volume:** 190   **Issue:** 4   **Pages:** 404-411   **DOI:** 10.1667/RR15020.1   **Published:** OCT 2018

Abstract: Experimental radiobiological studies in which the effects of ionizing radiation on a biological model are examined often highlight the biological aspects while missing detailed descriptions of the geometry, sample and dosimetric methods used. Such omissions can hinder the reproducibility and comparability of the experimental data. An application based on the Geant4 simulation toolkit was developed to design experiments using a biological solution placed in a microtube. The application was used to demonstrate the influence of the type of microtube, sample volume and energy of a proton source on the dose distribution across the sample, and on the mean dose in the whole sample. The results shown here are for samples represented by liquid water in the 0.4-, 1.5- and 2.0-ml microtubes irradiated with 20, 30 and 100 MeV proton beams. The results of this work demonstrate that the mean dose and homogeneity of the dose distribution within the sample strongly depend on all three parameters. Furthermore, this work shows how the dose uncertainty propagates into the scored primary DNA damages in plasmid DNA studies using agarase gel electrophoresis. This application is provided freely to assist users in verifying their experimental setup prior to the experiment. (C) 2018 by Radiation Research Society

Accession Number: WOS:000446180500007

PubMed ID: 30016217

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Record 45 of 214

Title: Survey of Grapevine Pinot gris virus in certified grapevine stocks in Ukraine

Author(s): Eichmeier, A (Eichmeier, Ales); Penazova, E (Penazova, Eliska); Muljukina, N (Muljukina, Nina)

Source: EUROPEAN JOURNAL OF PLANT PATHOLOGY   **Volume:** 152   **Issue:** 2   **Pages:** 555-560   **DOI:** 10.1007/s10658-018-1497-5   **Published:** OCT 2018

Abstract: Eighteen grapevine mother plants used by nurseries for propagation in Ukraine were tested for the presence of Grapevine Pinot gris virus (GPGV) and other viruses by simplex and multiplex RT-PCR (reverse transcription polymerase chain reaction). GPGV was found in 10 grapevines, which were also co-infected with Grapevine virus A (GVA) and Grapevine fleck virus (GFkV). We sequenced codingregions of the movement and coat protein and a region of the RdRp domain in twelve isolates. Phylogenetic analyses of the two genes revealed that the Ukrainian GPGV isolates grouped with previously described asymptomatic isolates. This study provides the first detailed survey of GPGV occurrence in Ukraine.

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Record 46 of 214

Title: Transcriptome reprogramming due to the introduction of a barley telosome into bread wheat affects more barley genes than wheat

Author(s): Rey, E (Rey, Elodie); Abrouk, M (Abrouk, Michael); Keeble-Gagnere, G (Keeble-Gagnere, Gabriel); Karafiatova, M (Karafiatova, Miroslava); Vrana, J (Vrana, Jan); Balzergue, S (Balzergue, Sandrine); Soubigou-Taconnat, L (Soubigou-Taconnat, Ludivine); Brunaud, V (Brunaud, Veronique); Martin-Magniette, ML (Martin-Magniette, Marie-Laure); Endo, TR (Endo, Takashi R.); Bartos, J (Bartos, Jan); Appels, R (Appels, Rudi); Dolezel, J (Dolezel, Jaroslav)

Group Author(s): Int Wheat Genome Sequencing Cons

Source: PLANT BIOTECHNOLOGY JOURNAL   **Volume:** 16   **Issue:** 10   **Pages:** 1767-1777   **DOI:** 10.1111/pbi.12913   **Published:** OCT 2018

Abstract: Despite a long history, the production of useful alien introgression lines in wheat remains difficult mainly due to linkage drag and incomplete genetic compensation. In addition, little is known about the molecular mechanisms underlying the impact of foreign chromatin on plant phenotype. Here, a comparison of the transcriptomes of barley, wheat and a wheat-barley 7HL addition line allowed the transcriptional impact both on 7HL genes of a non-native genetic background and on the wheat gene complement as a result of the presence of 7HL to be assessed. Some 42% (389/923) of the 7HL genes assayed were differentially transcribed, which was the case for only 3% (960/35301) of the wheat gene complement. The absence of any transcript in the addition line of a suite of chromosome 7A genes implied the presence of a 36 Mbp deletion at the distal end of the 7AL arm; this deletion was found to be in common across the full set of Chinese Spring/Betzes barley addition lines. The remaining differentially transcribed wheat genes were distributed across the whole genome. The up-regulated barley genes were mostly located in the proximal part of the 7HL arm, while the down-regulated ones were concentrated in the distal part; as a result, genes encoding basal cellular functions tended to be transcribed, while those encoding specific functions were suppressed. An insight has been gained into gene transcription in an alien introgression line, thereby providing a basis for understanding the interactions between wheat and exotic genes in introgression materials.

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PubMed ID: 29510004

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Record 47 of 214

Title: Stabilization of two coordinate tetrylene by borylamide ligand

Author(s): Aman, M (Aman, Michal); Mrozek, O (Mrozek, Ondrej); Dostal, L (Dostal, Libor); Ruzickova, Z (Ruzickova, Zdenka); Jambor, R (Jambor, Roman)

Source: JOURNAL OF ORGANOMETALLIC CHEMISTRY   **Volume:** 872   **Pages:** 1-7   **DOI:** 10.1016/j.jorganchem.2018.07.020   **Published:** OCT 1 2018

Abstract: Here we report the synthesis of aminoborane HN(BCy2) (C6H3-2,6-Me-2) (1) (Cy = cyclohexyl), that was successfully deprotonated and its lithium salt {LiN(BCy2) (C6H3-2,6-Me-2)}(2) (2) has been characterised. The borylamide ligand -N(BCy2) (C6H3-2,6-Me-2) was used for the preparation of N -> Sn coordinated stannylene [2,6-(Me2NCH2)(2)C6H3]Sn [N(BCy2) (C6H3-2,6-Me-2)] (3) and two coordinate tetrylenes {E [N(BCy2) (C6H3-2,6-Me-2)](2)} (E = Sn (4), Pb (5)). Experimental and theoretical studies suggested sigma character of E-N bonds without additional N(p)-> E(p) donation as the result of the preference of N(p)-> B(p) donation in 4 and 5. DFT studies on 4 and 5 also reveal theirs HOMO to exhibit E lone pair character and theirs LUMO to include p-orbital character located on metal atoms E. (C) 2018 Elsevier B.V. All rights reserved.

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Title: Big Data for Internet of Things: A Survey

Author(s): Ge, M (Ge, Mouzhi); Bangui, H (Bangui, Hind); Buhnova, B (Buhnova, Barbora)

Source: FUTURE GENERATION COMPUTER SYSTEMS-THE INTERNATIONAL JOURNAL OF ESCIENCE **Volume:** 87 **Pages:** 601-614 **DOI:** 10.1016/j.future.2018.04.053 **Published:** OCT 2018

Abstract: With the rapid development of the Internet of Things (IoT), Big Data technologies have emerged as a critical data analytics tool to bring the knowledge within IoT infrastructures to better meet the purpose of the IoT systems and support critical decision making. Although the topic of Big Data analytics itself is extensively researched, the disparity between IoT domains (such as healthcare, energy, transportation and others) has isolated the evolution of Big Data approaches in each IoT domain. Thus, the mutual understanding across IoT domains can possibly advance the evolution of Big Data research in IoT.
In this work, we therefore conduct a survey on Big Data technologies in different IoT domains to facilitate and stimulate knowledge sharing across the IoT domains. Based on our review, this paper discusses the similarities and differences among Big Data technologies used in different IoT domains, suggests how certain Big Data technology used in one IoT domain can be re-used in another IoT domain, and develops a conceptual framework to outline the critical Big Data technologies across all the reviewed IoT domains. (C) 2018 Elsevier B.V. All rights reserved.

Accession Number: WOS:000437997500050

Title: Recent trends and open questions in grain boundary segregation

Author(s): Lejcek, P (Lejcek, Pavel); Vsianska, M (Vsianska, Monika); Sob, M (Sob, Mojmir)

Source: JOURNAL OF MATERIALS RESEARCH **Volume:** 33 **Issue:** 18 **Pages:** 2647-2660 **DOI:** 10.1557/jmr.2018.230 **Published:** SEP 28 2018

Abstract: Recently, significant progress in the field of grain boundary segregation was achieved, for example, in better understanding and modeling the stabilization of nanocrystalline structures by grain boundary segregation, searching for more advanced approaches to theoretical calculation of segregation energies and development of the complexion approach. Nevertheless, with each progress, new important questions appear which need to be solved. Here, we focus on two basic questions appearing recently: How can be the experimental results on the grain boundary segregation compared reliably to their theoretical counterparts? Is the preferred segregation site of a solute in the grain boundary core substitutional or interstitial? We also show that the entropy of grain boundary segregation is a very important quantity which cannot be neglected in thermodynamic considerations as it plays a crucial role, for example, in prediction of thermodynamic characteristics of grain boundary segregation and in the preference of the segregation site at the boundary.

Accession Number: WOS:000446676400001

Title: Coassembly of Poly(N-isopropylacrylamide) with Dodecyl and Carboxyl Terminal Groups with Cationic Surfactant: Critical Comparison of Experimental and Simulation Data

Author(s): Fanova, A (Fanova, Anastasiia); Sindelka, K (Sindelka, Karel); Uchman, M (Uchman, Mariusz); Limpouchova, Z (Limpouchova, Zuzana); Filippov, SK (Filippov, Sergey K.); Pispas, S (Pispas, Stergios); Prochazka, K (Prochazka, Karel); Stepanek, M (Stepanek, Miroslav)

Source: MACROMOLECULES **Volume:** 51 **Issue:** 18 **Pages:** 7295-7308 **DOI:** 10.1021/acs.macromol.8b01161 **Published:** SEP 25 2018

Abstract: Comicellization of poly(N-isopropylacrylamide) with dodecyl and carboxyl terminal groups (mPNIPAm) with cationic surfactant N-dodecylpyridinium chloride was studied by scattering techniques (light scattering, SAXS), isothermal titration calorimetry, fluorescence spectroscopy, and coarse-grained simulations using dissipative particle dynamics (DPD) as a function of charge ratio of N-dodecylpyridinium (DP+) ions to mPNIPAm terminal carboxylate groups, Z = [DP+]/[COO-]. While both experimental results and DPD data indicate that up to Z = 2 tails of the surfactant enter and swell the dodecyl core of mPNIPAm micelles, the further increase in the size of the core for Z > 2 caused by the dehydration and collapse of inner parts of PNIPAm chains observed by SAXS is not reproduced by DPD simulations. Nevertheless, the study demonstrates that the simplified coarse-grained model can account for hydrogen bonding and elucidate the mechanism of comicellization. The study shows that the electrostatic interactions modify appreciably the behavior of mPNIPAm, but the assembly with cationic surfactant is governed by hydrophobic interactions.

Accession Number: WOS:000445971800031

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Record 51 of 214
Title: AA- and ABA-stacked carbon nitride (C3N4): novel photocatalytic water splitting solar-to-hydrogen energy conversion
Author(s): Reshak, AH (Reshak, A. H.)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 20 **Issue:** 35 **Pages:** 22972-22979 **DOI:** 10.1039/c8cp02898b **Published:** SEP 21 2018

Abstract: We report the development of the C3N4 structure by integrating two different structures: (i) two identical layers as AA-stacked C3N4 and (ii) intercalating one different layer between two identical layers as ABA-stacked C3N4. This in turn endows C3N4 with significantly promoted charge migration, up-shifted conduction-band (CB) level, enhanced CB potential from -0.89 eV (AA-stacked C3N4) to -1.03 eV (ABA-stacked C3N4), broadened band gap as well as enhanced surface area, all of which favor the enhancement of the photocatalytic performance. The optical absorption level exhibited significant enhancement in the visible light region when shifting from AA-stacked C3N4 to ABA-stacked C3N4, where the absorption edge moves from = 508.1 = 454.1 nm. This corresponds to the direct optical band gap of 2.44 eV 2.73 eV, which is well matched with the solar spectrum and the sufficient negative CB potential for H+/H-2 reduction. Based on these results, we can conclude that AA-stacked and ABA-stacked C3N4 satisfies all the requirements to be efficient photocatalysts. This study will significantly improve the search efficiency and considerably aid the experimentalists in the exploration of novel photocatalysts.
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PubMed ID: 30156220
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Record 52 of 214
Title: The black hole retention fraction in star clusters
Author(s): Pavlik, V (Pavlik, Vaclav); Jerabkova, T (Jerabkova, Tereza); Kroupa, P (Kroupa, Pavel); Baumgardt, H (Baumgardt, Holger)
Source: ASTRONOMY & ASTROPHYSICS **Volume:** 617 **Article Number:** A69 **DOI:** 10.1051/0004-6361/201832919 **Published:** SEP 19 2018

Abstract: Context. Recent research has been constraining the retention fraction of black holes (BHs) in globular clusters by comparing the degree of mass segregation with N-body simulations. They are consistent with an upper limit of the retention fraction being 50% or less.
Aims. In this work, we focus on direct simulations of the dynamics of BHs in star clusters. We aim to constrain the effective distribution of natal kicks that BHs receive during supernova (SN) explosions and to estimate the BH retention fraction.
Methods. We used the collisional N-body code nbody6 to measure the retention fraction of BHs for a given set of parameters, which are: the initial mass of a star cluster, the initial half-mass radius, and sigma(BH), which sets the effective Maxwellian BH velocity kick distribution. We compare these direct N-body models with our analytic estimates and newest observational constraints.
Results. The numerical simulations show that for the one-dimensional velocity kick dispersion sigma BH < 50 km s(-1), clusters with radii of 2 pc and that are initially more massive than 5 x 10(3) M-circle dot retain more than 20% of BHs within their half-mass radii. Our simple analytic model yields a number of retained BHs that is in good agreement with the N-body models. Furthermore, the analytic estimates show that ultra-compact dwarf galaxies should have retained more than 80% of their BHs for sigma BH <= 190 km s(-1). Although our models do not contain primordial binaries, in the most compact clusters with 10(3) stars, we have found evidence of delayed SN explosions producing a surplus of BHs compared to the IMF due to dynamically formed binary stars. These cases do not occur in the more populous or expanded clusters.
Accession Number: WOS:000444935100001
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Record 53 of 214
Title: Filter-Aided Sample Preparation Procedure for Mass Spectrometric Analysis of Plant Histones
Author(s): Ledvinova, D (Ledvinova, Dominika); Mikulasek, K (Mikulasek, Kamil); Kucharikova, H (Kucharikova, Hana); Brabencova, S (Brabencova, Sylva); Fojtova, M (Fojtova, Miloslava); Zdrahal, Z (Zdrahal, Zbynek); Lochmanova, G (Lochmanova, Gabriela)
Source: FRONTIERS IN PLANT SCIENCE **Volume:** 9 **Article Number:** 1373 **DOI:** 10.3389/fpls.2018.01373 **Published:** SEP 19 2018

Abstract: Characterization of histone post-translational modifications (PTMs) is still challenging, and robust histone sample preparation is essential for convincing evaluation of PTMs by mass spectrometry. An effective protocol for extracting plant histone proteins must also avoid excessive co-extraction of the numerous potential interfering compounds, including those related to secondary metabolism. Currently, the co-existence of histone marks is addressed mostly by shotgun proteomic analysis following chemical derivatization of histone lysine residues. Here, we report a straightforward approach for plant histone sample preparation for mass spectrometry, based on filter-aided sample preparation coupled with histone propionylation. The approach offers savings in sample handling and preparation time, enables removal of interfering compounds from the sample, and does not require either precipitation or dialysis of histone extract. We show the comparison of two protocol variants for derivatization of histone proteins, in-solution propionylation in the vial and propionylation on the filter unit. For both protocols, we obtained identical abundances of post-translationally modified histone peptides. Although shorter time is required for histone protein labeling on the filter unit, in-solution derivatization slightly outweighed filter-based variant by lower data variability. Nevertheless, both protocol variants appear to be efficient and convenient approach for preparation of plant histones for mass spectrometric analysis.
Accession Number: WOS:000444989900002
PubMed ID: 30283482
ISSN: 1664-462X

Record 54 of 214
Title: Why is Benzene Unique? Screening Magnetic Properties of C6H6 Isomers
Author(s): Janda, T (Janda, Tomas); Foroutan-Nejad, C (Foroutan-Nejad, Cina)
Source: CHEMPHYSCHEM **Volume:** 19 **Issue:** 18 **Pages:** 2357-2363 **DOI:** 10.1002/cphc.201800364 **Published:** SEP 18 2018

Abstract: Magnetic properties are commonly used to identify new aromatic molecules because it is generally believed that magnetization and energetic stability are correlated. To verify the potential correlation between the energy and magnetic response properties, we examined a set of 198 isomers of C6H6. The energy and magnetic properties of these molecules can be directly compared with no need to invoke any arbitrary reference state because the studied systems are all isomers. Benzene is the global minimum on the potential energy surface of C6H6, 35kcalmol(-1) lower in energy than the second most stable isomer, fulvene. Unlike its electronic energy, isotropic magnetizability of benzene is slightly lower than the average magnetizability of its isomers. Altogether, 44 isomers of C6H6 were identified to have more negative magnetic susceptibility than benzene but were between 67.0 to 168.6kcalmol(-1) higher in energy than benzene. However, benzene is unique in two ways. Analyzing the paramagnetic contribution to the magnetic susceptibility as originally suggested by Bilde and Hansen (Mol. Phys., 1997, 92, 237) revealed that 53molecules have lower paramagnetic susceptibility than benzene but among monocyclic systems benzene has the least paramagnetic susceptibility. Furthermore, benzene has the largest out-of-plane magnetic susceptibility that originates from the strongest ring current among all studied species.
Accession Number: WOS:000444411500011
PubMed ID: 29799650
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eISSN: 1439-7641

Record 55 of 214
Title: Thermodynamic model for a reversible desalination cycle using weak polyelectrolyte hydrogels

Author(s): Rud, O (Rud, Oleg); Borisov, O (Borisov, Oleg); Kosovan, P (Kosovan, Peter)
Abstract: The recently proposed use of hydrogels for water desalination is based on the decrease of salt concentration in the gel upon compression. In the first experiments, desalination cycles using hydrogels involved an irreversible mixing step, which inevitably reduced the thermodynamic efficiency. This approach could become competitive with membrane-based desalination methods if it could work close to maximum thermodynamic efficiency. In this work, we develop a thermodynamic model for compression of weak polyelectrolyte hydrogels in open and closed systems. We use this model to design a fully reversible desalination cycle which can, in principle, achieve maximum thermodynamic efficiency.
We also show that compressing weak polyelectrolyte hydrogels at low salinity decreases their ionization, thereby leading to a non-monotonic dependence of salt concentration on the gel compression. Therefore, our model shows how to redesign the desalination cycle when using weak polyelectrolytes at low salinities.

Title: Toll-Like Receptor Evolution in Birds: Gene Duplication, Pseudogenization, and Diversifying Selection
Author(s): Velova, H (Velova, Hana); Gutowska-Ding, MW (Gutowska-Ding, Maria W.); Burt, DW (Burt, David W.); Vinkler, M (Vinkler, Michal)
Abstract: Toll-like receptors (TLRs) are key sensor molecules in vertebrates triggering initial phases of immune responses to pathogens. The avian TLR family typically consists of ten receptors, each adapted to distinct ligands. To understand the complex evolutionary history of each avian TLR, we analyzed all members of the TLR family in the whole genome assemblies and target sequence data of 63 bird species covering all major avian clades. Our results indicate that gene duplication events most probably occurred in TLR1 before synapsids diversified from sauropsids. Unlike mammals, ssRNA-recognizing TLR7 has duplicated independently in several avian taxa, while flagellin-sensing TLR5 has pseudogenized multiple times in bird phylogeny. Our analysis revealed stronger positive, diversifying selection acting in TLR5 and the three-domain TLRs (TLR10 [TLR1A], TLR1 [TLR1B], TLR2A, TLR2B, TLR4) that face the extracellular space and bind complex ligands than in single-domain TLR15 and endosomal TLRs (TLR3, TLR7, TLR21). In total, 84 out of 306 positively selected sites were predicted to harbor substitutions dramatically changing the amino acid physicochemical properties. Furthermore, 105 positively selected sites were located in the known functionally relevant TLR regions. We found evidence for convergent evolution acting between birds and mammals at 54 of these sites. Our comparative study provides a comprehensive insight into the evolution of avian TLR genetic variability. Besides describing the history of avian TLR gene gain and gene loss, we also identified candidate positions in the receptors that have been likely shaped by direct molecular host-pathogen coevolutionary interactions and most probably play key functional roles in birds.
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Title: Increased Expression of Maturation Promoting Factor Components Speeds Up Meiosis in Oocytes from Aged Females
Author(s): Koncicka, M (Koncicka, Marketa); Tetkova, A (Tetkova, Anna); Jansova, D (Jansova, Denisa); Del Llano, E (Del Llano, Edgar); Gahurova, L (Gahurova, Lenka); Kracmarova, J (Kracmarova, Jana); Prokesova, S (Prokesova, Sarka); Masek, T (Masek, Tomas); Pospisek, M (Pospisek, Martin); Bruce, AW (Bruce, Alexander W.); Kubelka, M (Kubelka, Michal); Susor, A (Susor, Andrej)
Abstract: The rate of chromosome segregation errors that emerge during meiosis I in the mammalian female germ line are known to increase with maternal age; however, little is known about the underlying molecular mechanism. The objective of this study was to analyze meiotic progression of mouse oocytes in relation to maternal age. Using the mouse as a model system, we analyzed the timing of nuclear envelope breakdown and the morphology of the nuclear lamina of oocytes obtained from young (2 months old) and aged females (12 months old). Oocytes obtained from older females display a significantly faster progression through meiosis I compared to the ones obtained from younger females. Furthermore, in oocytes from aged females, lamin A/C structures exhibit rapid phosphorylation and dissociation. Additionally, we also found an increased abundance of MPF components and increased translation of factors controlling translational activity in the oocytes of aged females. In conclusion, the elevated MPF activity observed in aged female oocytes affects precocious meiotic processes that can multifactorially contribute to chromosomal errors in meiosis I.
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Title: Transmission Optimization Metrics Setup Issues in the Field of Time Constrained Communications
Author(s): Vondrous, O (Vondrous, Ondrej); Kocur, Z (Kocur, Zbynek); Hrad, J (Hrad, Jaromir)
Abstract: This article introduces a new approach in the field of network optimization based on Transmission Optimization Metric (TOM), which is aimed at improving traffic flow continuity and increasing the chances for traffic flow sustainability in a way that helps to minimize inter-packet gaps. The work is mainly focused on harsh transmission conditions in narrow-band networks. Finally, the presented approach has impact on better resource allocation as fewer attempts are necessary for successful completion of a transmission. A significant part of the article deals with parameterization of coefficients used by the TOM optimization method. Examples of analysis for several topologies of narrow-band wireless networks based on CSMA/CA and TDMA protocols are used to demonstrate various issues related to proper setting of parameters. The introduced TOM metric has the potential to become a standard for optimization, for example, in sensor networks that are characterized by the specific nature of data traffic.
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Title: Mass dependence of vector meson photoproduction off protons and nuclei within the energy-dependent hot-spot model
Author(s): Cepila, J (Cepila, J.); Contreras, JG (Contreras, J. G.); Krelina, M (Krelina, M.); Takaki, JDT (Takaki, J. D. Tapia)
Abstract: We study the photoproduction of vector mesons off proton and off nuclear targets. We work within the colour dipole model in an approach that includes subnucleon degrees of freedom, so-called hot spots, whose positions in the impact-parameter plane change event-by-event. The key feature of our model is that the number of hot spots depends on the energy of the photon-target interaction. Predictions are presented for exclusive and dissociative production of rho(0), J/psi, and Upsilon(1S) off protons, as well as for coherent and

incoherent photoproduction of rho(0) off nuclear targets, where Xe, Au, and Pb nuclei are considered. We find that the mass dependence of dissociative production off protons as a function of the energy of the interaction provides a further handle to search for saturation effects at HERA, the LHC and future colliders. We also find that the coherent photonuclear production of rho(0) is sensitive to fluctuations in the subnucleon degrees of freedom at RHIC and LHC energies. (C) 2018 The Author(s). Published by Elsevier B.V.

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Record 60 of 214

Title: Functional Analysis of Novicidin Peptide: Coordinated Delivery System for Zinc via Schiff Base Ligand

Author(s): Milosavljevic, V (Milosavljevic, Vedran); Haddad, Y (Haddad, Yazan); Moulick, A (Moulick, Amitava); Buchtelova, H (Buchtelova, Hana); Guran, R (Guran, Roman); Pospisil, T (Pospisil, Tomas); Stokowa-Soltys, K (Stokowa-Soltys, Kamila); Heger, Z (Heger, Zbynek); Richtera, L (Richtera, Lukas); Kopel, P (Kopel, Pavel); Adam, V (Adam, Vojtech)

Source: BIOCONJUGATE CHEMISTRY **Volume:** 29 **Issue:** 9 **Pages:** 2954-2969 **DOI:** 10.1021/acs.bioconjchem.8b00370 **Published:** SEP 2018

Abstract: Novicidin (NVC), is a membrane-penetrating peptide, which forms a stable complex with Zn-Schiff base with interesting antitumor selectivity. We studied NVC derivatives to determine functional roles of key amino acids in toxicity, helicity, and binding of the Zn-Schiff base complex. Trimmed derivatives highlighted the role of peptide length and helicity in toxicity and membrane penetration. The removal of Lys from position 1 and 2 strongly increases the ability to disrupt the membranes. The trimming of the N-terminal residues significantly increases the stability of peptide helicity enhancing penetrating properties. Gly residue derivatives undermined a role of peptide bending in membrane penetration and toxicity. After the substitution of the central Gly derivatives with Ile or Lys, the peptides retained toxicity. These results illustrate the minor role of central helix bending in NVC toxicity. Binding-site-peptide derivatives identified His residue as the sole Zn-Schiff base binding site and eliminated the role of other aromatic residues.

Accession Number: WOS:000445439500011

PubMed ID: 30086240

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ISSN: 1043-1802

Record 61 of 214

Title: Molecular dynamics study of racemic mixtures: Solutions of ibuprofen and beta-cyclodextrin in methanol

Author(s): Skvara, J (Skvara, Jiri); Nezbeda, I (Nezbeda, Ivo)

Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 265 **Pages:** 791-796 **DOI:** 10.1016/j.molliq.2018.07.020 **Published:** SEP 1 2018

Abstract: Using a realistic all-atom interaction model, molecular dynamics simulations were carried out for five different setups of racemic mixtures of chiral molecules of ibuprofen and beta-cyclodextrin, and also of their solution in methanol. The setups included a pair of these molecules in vacuum, their mixture in the liquid phase, and the solution of ibuprofen in methanol in beta-cyclodextrin channels. Several structural properties have been evaluated to identify differences in the behavior of the (S) and (R) forms in the coordination shells of beta-cyclodextrin. It turns out that (R)-ibuprofen forms a more stable complex and also more easily penetrates the molecule of beta-cyclodextrin. At beta-cyclodextrin walls, (R)-ibuprofen forms preferably DOWN complex whereas (S) -ibuprofen prefers UP complex. The obtained results will serve as a benchmark for development of a coarse-grained model used to study the roles of the structure of molecules and of different intermolecular interactions in separation of racemic mixtures. (C) 2018 Elsevier B.V. All rights reserved.

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Record 62 of 214

Title: Aldo-keto reductase 1C3 (AKR1C3): a missing piece of the puzzle in the dinaciclib interaction profile

Author(s): Novotna, E (Novotna, Eva); Bukum, N (Bukum, Neslihan); Hofman, J (Hofman, Jakub); Flaxova, M (Flaxova, Michaela); Kouklikova, E (Kouklikova, Etela); Louvarova, D (Louvarova, Dagmar); Wsol, V (Wsol, Vladimir)

Source: ARCHIVES OF TOXICOLOGY **Volume:** 92 **Issue:** 9 **Pages:** 2845-2857 **DOI:** 10.1007/s00204-018-2258-0 **Published:** SEP 2018

Abstract: Dinaciclib is a multi-specific cyclin-dependent kinase (CDK) inhibitor with significant preclinical and clinical activity. It inhibits CDK1, CDK2, CDK5, CDK9 and CDK12 in the nanomolar range and exhibits potent antiproliferative effects on various cancers in vitro and in vivo. Aldo-keto reductases (AKR) and carbonyl reductases (CBR) are enzymes involved at the biosynthesis, intermediary metabolism and detoxification processes, but can also play a significant role in cancer resistance. Here, we report that dinaciclib is a strong inhibitor of aldo-keto reductase 1C3 (AKR1C3), an enzyme that is known to be an important regulator of cell proliferation and differentiation. AKR1C3 is overexpressed in a range of cancer types and is also involved in tumour cell resistance to anthracyclines. In our study, dinaciclib displayed tight-binding inhibition of human recombinant AKR1C3 (Ki(app) = 0.07 A mu M) and was also active at the cellular level (IC50 = 0.23 A mu M). Dinaciclib acts as a noncompetitive inhibitor with respect to daunorubicin and as an uncompetitive inhibitor with respect to the NADPH. In subsequent experiments, pretreatment with dinaciclib (0.1 A mu M) significantly sensitized AKR1C3-overexpressing anthracycline-resistant cancer cells to daunorubicin. In conclusion, our results indicate that dinaciclib may potentially increase the therapeutic efficacy and safety of anthracyclines by preventing anthracycline resistance and minimizing their adverse effects.

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PubMed ID: 29992508

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Record 63 of 214

Title: On the importance of being stable: evolutionarily frozen species can win in fluctuating environments

Author(s): Flegr, J (Flegr, Jaroslav); Ponizil, P (Ponizil, Petr)

Source: BIOLOGICAL JOURNAL OF THE LINNEAN SOCIETY **Volume:** 125 **Issue:** 1 **Pages:** 210-220 **DOI:** 10.1093/biolinnean/bly110 **Published:** SEP 2018

Abstract: The ability of organisms to respond adaptively to environmental changes (evolvability) is usually considered to be an important advantage in interspecific competition. It has been suggested, however, that evolvability could be a double-edged sword that could present a handicap in fluctuating environments. The authors of this counterintuitive idea have published only verbal models to support their claims. Here, we present the results of individual-based stochastic modelling of competition between two asexual species that differ only by their evolvability. They show that, in changeable environments, less evolvable species could outperform their more evolvable competitors in a broad area of a parameter space. Highly evolvable species prospered better nearly all the time; however, they sustained a higher probability of extinction during rare events of the rapid transient change of conditions. It explains why sexual species, with their reduced capacity to respond adaptively to local or temporal environmental changes, prevail in nearly all biotopes.

Accession Number: WOS:000442937000018

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ISSN: 0024-4066

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Record 64 of 214

Title: Effect of Si and Ge Surface Doping on the Be2C Monolayer: Case Study on Electrical and Optical Properties

Author(s): Naseri, M (Naseri, Mosayeb); Reshak, AH (Reshak, Ali H.); Boochani, A (Boochani, Arash); Rai, DP (Rai, D. P.); Matin, LF (Matin, Laleh Farhang); Solaymani, S (Solaymani, Shahram)

Abstract: The electronic and optical properties of X (Si, Ge) doped Be2C monolayer has been investigated using the all-electron full potential linear augmented plane wave (FP-LAPW+lo) method in a scalar relativistic version as embodied in the Wien2k code based on the density functional theory. Using cohesive energy calculation, it has been shown that the Si and Ge doped to Be2C monolayer have stable structures and the doping processes modified the direct band gaps. The calculated electronic band structure confirm the direct band gap nature since the conduction band minimum and the valence band maximum are located at the center of the Brillouin zone. The total and partial density of states help to gain further information regarding the hybridizations and the orbitals which control the energy band gap. The calculated optical properties help to gain deep insight into the electronic structure. Our calculated results indicate that the X (Si, Ge) doped Be2C monolayer can be have potential application in optoelectronics devices.

Accession Number: WOS:000442754000012

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Record 65 of 214

Title: The matrix-twin transition in a perfect Mg crystal: Ab initio study

Author(s): Kana, T (Kana, Tomas); Ostapovets, A (Ostapovets, Andriy); Paidar, V (Paidar, Vaclav)

Abstract: By means of ab initio calculations, we studied the matrix - twin transition in a perfect Mg crystal where the {10 (1) over bar2} plane is the twinning plane. The twinning transition is described by the shear of a suitable periodically repeated unit cell and by the atomic shuffling inside the unit cell. We found two hcp - hcp paths that can create the glide and reflection {10 (1) over bar2} twin boundary, respectively. Assuming a perfect hcp crystal, it turned out that the total energy profiles of both hcp - hcp paths are the same. We further pointed out the equivalence between the description of the matrix - twin transition in the frame of an orthorhombic and of a monoclinic unit cell, both containing four atoms. We have tracked the trajectories of the net atomic motion that are energetically very favorable. In addition, the effect of volume relaxation on the total energy profiles was investigated and its influence on the plastic deformation of Mg crystal was discussed.

Accession Number: WOS:000442061900011

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Record 66 of 214

Title: A gene transfer event suggests a long-term partnership between eustigmatophyte algae and a novel lineage of endosymbiotic bacteria

Author(s): Yurchenko, T (Yurchenko, Tatiana); Sevcikova, T (Sevcikova, Tereza); Pribyl, P (Pribyl, Pavel); El Karkouri, K (El Karkouri, Khalid); Klimes, V (Klimes, Vladimir); Amaral, R (Amaral, Raquel); Zbrankova, V (Zbrankova, Veronika); Kim, E (Kim, Eunsoo); Raoult, D (Raoult, Didier); Santos, LMA (Santos, Lilia M. A.); Elias, M (Elias, Marek)

Abstract: Rickettsiales are obligate intracellular bacteria originally found in metazoans, but more recently recognized as widespread endosymbionts of various protists. One genus was detected also in several green algae, but reports on rickettsialean endosymbionts in other algal groups are lacking. Here we show that several distantly related eustigmatophytes (coccoid algae belonging to Ochrophyta, Stramenopiles) are infected by Candidatus Phycorickettsia gen. nov., a new member of the family Rickettsiaceae. The genome sequence of Ca. Phycorickettsia trachydisci sp. nov., an endosymbiont of Trachydiscus minutus CCALA 838, revealed genomic features (size, GC content, number of genes) typical for other Rickettsiales, but some unusual aspects of the gene content were noted. Specifically, Phycorickettsia lacks genes for several components of the respiration chain, haem biosynthesis pathway, or c-di-GMP-based signalling. On the other hand, it uniquely harbours a six-gene operon of enigmatic function that we recently reported from plastid genomes of two distantly related eustigmatophytes and from various non-rickettsialean bacteria. Strikingly, the eustigmatophyte operon is closely related to the one from Phycorickettsia, suggesting a gene transfer event between the endosymbiont and host lineages in early eustigmatophyte evolution. We hypothesize an important role of the operon in the physiology of Phycorickettsia infection and a long-term eustigmatophyte-Phycorickettsia coexistence.

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PubMed ID: 29880910

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Record 67 of 214

Title: Robustness of Representative Signals Relative to Data Loss Using Atlas-Based Parcellations

Author(s): Gajdos, M (Gajdos, Martin); Vytvarova, E (Vytvarova, Eva); Fousek, J (Fousek, Jan); Lamos, M (Lamos, Martin); Mikl, M (Mikl, Michal)

Abstract: Parcellation-based approaches are an important part of functional magnetic resonance imaging data analysis. They are a necessary processing step for sorting data in structurally or functionally homogenous regions. Real functional magnetic resonance imaging datasets usually do not cover the atlas template completely; they are often spatially constrained due to the physical limitations of MR sequence settings, the inter-individual variability in brain shape, etc. When using a parcellation template, many regions are not completely covered by actual data. This paper addresses the issue of the area coverage required in real data in order to reliably estimate the representative signal and the influence of this kind of data loss on network analysis metrics. We demonstrate this issue on four datasets using four different widely used parcellation templates. We used two erosion approaches to simulate data loss on the whole-brain level and the ROI-specific level. Our results show that changes in ROI coverage have a systematic influence on network measures. Based on the results of our analysis, we recommend controlling the ROI coverage and retaining at least 60% of the area in order to ensure at least 80% of explained variance of the original signal.

Accession Number: WOS:000440763900004

PubMed ID: 29693205

Record 68 of 214

Title: Widespread evolutionary crosstalk among protein domains in the context of multi- domain proteins

Author(s): Jakubec, D (Jakubec, David); Kratochvil, M (Kratochvil, Miroslav); Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri)

Abstract: Domains are distinct units within proteins that typically can fold independently into recognizable three-dimensional structures to facilitate their functions. The structural and functional independence of protein domains is reflected by their apparent modularity in the context of multi-domain proteins. In this work, we examined the coupling of evolution of domain sequences co-occurring within multi-domain proteins to see if it proceeds independently, or in a coordinated manner. We used continuous information theory measures to assess the extent of correlated mutations among domains in multi-domain proteins from organisms across the tree of life. In all multi-domain architectures we examined, domains co-occurring within protein sequences had to some degree undergone concerted evolution. This finding challenges the notion of complete modularity and independence of protein domains, providing new perspective on the evolution of protein sequence and function.

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PubMed ID: 30169546

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ISSN: 1932-6203

Record 69 of 214

Title: Fluorination of Black Phosphorus-Will Black Phosphorus Burn Down in the Elemental Fluorine?

Author(s): Plutnar, J (Plutnar, Jan); Sturala, J (Sturala, Jiri); Mazanek, V (Mazanek, Vlastimil); Sofer, Z (Sofer, Zdenek); Pumera, M (Pumera, Martin)

Source: ADVANCED FUNCTIONAL MATERIALS **Volume:** 28 **Issue:** 35 **Article Number:** 1801438 **DOI:** 10.1002/adfm.201801438 **Published:** AUG 29 2018

Abstract: Black phosphorus (BP) represents a promising tunable bandgap alternative to graphene and other 2D materials in the field of semiconductors. However, its reactivity toward covalent modification of its surface (as a key to its bandgap adjustment) is scarcely reported. Here a method of covalent modification of BP involving reaction with fluorine is reported. Other allotropes of phosphorus are known to react violently with fluorine resulting in its complete burning down and formation of gaseous phosphorus pentafluoride. The results of our fluorination experiments conducted in analogy to the procedures used for fluorination of graphene indicate a successful binding of fluorine to BP. This route of modification of BP opens new possible ways toward covalent modification of the surface of this promising material.

Accession Number: WOS:000442731200005

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ISSN: 1616-301X

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Record 70 of 214

Title: Functionally specific binding regions of microtubule-associated protein 2c exhibit distinct conformations and dynamics

Author(s): Melkova, K (Melkova, Katerina); Zapletal, V (Zapletal, Vojtech); Jansen, S (Jansen, Severine); Nomilner, E (Nomilner, Erik); Zachrdla, M (Zachrdla, Milan); Hritz, J (Hritz, Jozef); Novacek, J (Novacek, Jiri); Zweckstetter, M (Zweckstetter, Markus); Jensen, MR (Jensen, Malene R.); Blackledge, M (Blackledge, Martin); Zidek, L (Zidek, Lukas)

Source: JOURNAL OF BIOLOGICAL CHEMISTRY **Volume:** 293 **Issue:** 34 **Pages:** 13297-13309 **DOI:** 10.1074/jbc.RA118.001769 **Published:** AUG 24 2018

Abstract: Microtubule-associated protein 2c (MAP2c) is a 49-kDa intrinsically disordered protein regulating the dynamics of microtubules in developing neurons. MAP2c differs from its sequence homologue Tau in the pattern and kinetics of phosphorylation by cAMP-dependent protein kinase (PKA). Moreover, the mechanisms through which MAP2c interacts with its binding partners and the conformational changes and dynamics associated with these interactions remain unclear. Here, we used NMR relaxation and paramagnetic relaxation enhancement techniques to determine the dynamics and long-range interactions within MAP2c. The relaxation rates revealed large differences in flexibility of individual regions of MAP2c, with the lowest flexibility observed in the known and proposed binding sites. Quantitative conformational analyses of chemical shifts, small-angle X-ray scattering (SAXS), and paramagnetic relaxation enhancement measurements disclosed that MAP2c regions interacting with important protein partners, including Fyn tyrosine kinase, plectin, and PKA, adopt specific conformations. High populations of polyproline II and alpha-helices were found in Fyn- and plectin-binding sites of MAP2c, respectively. The region binding the regulatory subunit of PKA consists of two helical motifs bridged by a more extended conformation. Of note, although MAP2c and Tau did not differ substantially in their conformations in regions of high sequence identity, we found that they differ significantly in long-range interactions, dynamics, and local conformation motifs in their N-terminal domains. These results highlight that the N-terminal regions of MAP2c provide important specificity to its regulatory roles and indicate a close relationship between MAP2c's biological functions and conformational behavior.

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PubMed ID: 29925592

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Zidek, Lukas	D-7112-2012	

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Record 71 of 214

Title: The triple system HD 150136: From periastron passage to actual masses

Author(s): Mahy, L (Mahy, L.); Gosset, E (Gosset, E.); Manfroid, J (Manfroid, J.); Nitschelm, C (Nitschelm, C.); Herve, A (Herve, A.); Semaan, T (Semaan, T.); Sana, H (Sana, H.); Le Bouquin, JB (Le Bouquin, J. -B.); Toonen, S (Toonen, S.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 616 **Article Number:** A75 **DOI:** 10.1051/0004-6361/201832810 **Published:** AUG 21 2018

Abstract: Context. The triple system HD 150136 is composed of an O3 V((f*))-O3.5 V((f(+))) primary, of an O5.5-6 V((f)) secondary, and of a more distant O6.5-7 V((f)) tertiary. The latter component went through periastron in 2015-2016, an event that will not occur again within the next eight years.

Aims. We aim to analyse the tertiary periastron passage to determine the orbital properties of the outer system, to constrain its inclination and its eccentricity, and to determine the actual masses of the three components of the system.

Methods. We conducted an intensive spectroscopic monitoring of the periastron passage of the tertiary component and combined the outcoming data with new interferometric measurements. This allows us to derive the orbital solution of the outer orbit in three-dimensional space. We also obtained the light curve of the system to further constrain the inclination of the inner binary.

Results. We determine an orbital period of 8.61 +/- 0.02 years, an eccentricity of 0.682 +/- 0.002, and an inclination of 106.18 +/- 0.14 degrees for the outer orbit. The actual masses of the inner system and of the tertiary object are 72.32(-8.49)(+8.45) M-circle dot and 15.54(-4.97)(+4.96) M-circle dot, respectively. From the mass of the inner system and accounting for the known mass ratio between the primary and the secondary, we determine actual masses of 42.81 M-circle dot and 29.51 M-circle dot for the primary and the secondary components, respectively. We infer, from the different mass ratios and the inclination of the outer orbit, an inclination of 62.4 degrees for the inner system. This value is confirmed by photometry. Grazing eclipses and ellipsoidal variations are detected in the light curve of HD 150136. We also compute the distance of the system to 1.096 +/- 0.274 kpc.

Conclusions. By combining spectroscopy, interferometry, and photometry, HD 150136 offers us a unique chance to compare theory and observations. The masses estimated through our analysis are smaller than those constrained by evolutionary models. The formation of this triple system suggests similar ages for the three components within the errorbars. Finally, we show that Lidov-Kozai cycles have no effect on the evolution of the inner binary, which suggests that the latter will experience mass transfer leading to a merger of the two stars.

Accession Number: WOS:000442540500001

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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ISSN: 1432-0746

Record 72 of 214

Title: Sequencing of Treponema pallidum subsp pallidum from isolate UZ1974 using Anti-Treponemal Antibodies Enrichment: First complete whole genome sequence obtained directly from human clinical material

Author(s): Grillova, L (Grillova, Linda); Giacani, L (Giacani, Lorenzo); Mikalova, L (Mikalova, Lenka); Strouhal, M (Strouhal, Michel); Strnadel, R (Strnadel, Radim); Marra, C (Marra, Christina); Centurion-Lara, A (Centurion-Lara, Arturo); Poveda, L (Poveda, Lucy); Russo, G (Russo, Giancarlo); Cejkova, D (Cejkova, Darina); Vasku, V (Vasku, Vladimir); Oppelt, J (Oppelt, Jan); Smajs, D (Smajs, David)

Source: PLOS ONE **Volume:** 13 **Issue:** 8 **Article Number:** e0202619 **DOI:** 10.1371/journal.pone.0202619 **Published:** AUG 21 2018

Abstract: Treponema pallidum subsp. pallidum (TPA) is the infectious agent of syphilis, a disease that infects more than 5 million people annually. Since TPA is an uncultivable bacterium, most of the information on TPA genetics comes from genome sequencing and molecular typing studies. This study presents the first complete TPA genome (without sequencing gaps) of clinical isolate (UZ1974), which was obtained directly from clinical material, without multiplication in rabbits. Whole genome sequencing was performed using a newly developed Anti-Treponemal Antibody Enrichment technique combined with previously reported Pooled Segment Genome Sequencing. We identified the UW074B genome, isolated from a sample previously propagated in rabbits, to be the closest relative of the UZ1974 genome and calculated the TPA mutation rate as $2.8 \times 10^{(-10)}$ per site per generation.

Accession Number: WOS:000442284500011
PubMed ID: 30130365
Author Identifiers:

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Cejkova, Darina		0000-0002-6989-6330

ISSN: 1932-6203

Record 73 of 214

Title: Activation/Inactivation Role of Ionic Liquids on Formate Dehydrogenase from Pseudomonas sp 101 and Its Mutated Thermostable Form

Author(s): D'Oronzo, E (D'Oronzo, Erica); Secundo, F (Secundo, Francesco); Minofar, B (Minofar, Babak); Kulik, N (Kulik, Natallia); Pometun, AA (Pometun, Anastasia A.); Tishkov, VI (Tishkov, Vladimir I.)

Source: CHEMCATCHEM **Volume:** 10 **Issue:** 15 **Pages:** 3247-3259 **DOI:** 10.1002/cctc.201800145 **Published:** AUG 13 2018

Abstract: Ionic liquids (ILs) are used in numerous research areas including biocatalysis. The effect of ILs/water mixture on the activity of wild type and a more thermally and chemically stable mutant (SM4) of a specific formate dehydrogenases (PseFDH, EC1.2.1.2) were studied experimentally and by molecular dynamics (MD) simulations. The ILs investigated were [Mmim][Me2PO4], [Bmim][Br], [Bmim][CH3SO3], [Bmim][BF4], [Bmim][AcO], and it was found that low concentrations (optimally 2.5%) of some ILs increased (up to 42%) the activity of the SM4 FDH but not of the WT FDH. Using intrinsic fluorescence to calculate Stern-Volmer constants and thermodynamic parameters, we have studied protein conformational changes caused by ILs for both enzymes. Kinetic analyses allowed us to shed light on the mechanism of activation by 2.5% [Bmim][BF4] on the mutant enzyme. MD simulation provided evidences of a molecular basis of different enzyme activities in ILs that well correlated with the experimental data.

Accession Number: WOS:000442208200009
Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Secundo, Francesco		0000-0002-7052-9634

ISSN: 1867-3880
eISSN: 1867-3899

Record 74 of 214

Title: Isocorroles as Homoaromatic NIR-Absorbing Chromophores: A First Quantum Chemical Study

Author(s): Foroutan-Nejad, C (Foroutan-Nejad, Cina); Larsen, S (Larsen, Simon); Conradie, J (Conradie, Jeanet); Ghosh, A (Ghosh, Abhik)

Source: SCIENTIFIC REPORTS **Volume:** 8 **Article Number:** 11952 **DOI:** 10.1038/s41598-018-29819-3 **Published:** AUG 10 2018

Abstract: Density functional theory calculations of magnetically induced current densities have revealed high diatropic ring currents in unsubstituted isocorrole consistent with homoaromatic character. An examination of the Kohn-Sham molecular orbitals showed clear evidence of homoconjugative interactions in four occupied p-type molecular orbitals as well as in the LUMO. Remarkably, substituents at the saturated meso position were found to exert a dramatic influence on the overall current density pattern. Thus, whereas bis(trimethylsilyl)-substitution strongly enhanced the peripheral diatropic current (consistent with enhanced homoaromaticity), difluoro-substitution engendered a strong, net paratropic current (consistent with antihomoaromaticity). In this respect, isocorroles stand in sharp contrast to benzenoid aromatics, for which substituents typically exert a small influence on the current density distribution.

Accession Number: WOS:000441299000002
PubMed ID: 30097587
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Conradie, Jeanet		0000-0002-8120-6830

ISSN: 2045-2322

Record 75 of 214

Title: Synthesis, Crystal Structure, and Optical Gap of Two-Dimensional Halide Solid Solutions CsPb2 (Cl1-xBrx)(5)

Author(s): Chen, YB (Chen, Yibao); Molokeev, MS (Molokeev, Maxim S.); Atuchin, VV (Atuchin, Victor V.); Reshak, AH (Reshak, Ali H.); Auluck, S (Auluck, Sushil); Alahmed, ZA (Alahmed, Zeyad A.); Xia, ZG (Xia, Zhiguo)

Source: INORGANIC CHEMISTRY **Volume:** 57 **Issue:** 15 **Pages:** 9531-9537 **DOI:** 10.1021/acs.inorgchem.8b01572 **Published:** AUG 6 2018

Abstract: Exploring new perovskite-related solid-state materials and the investigating composition-dependent structural and physical properties are highly important for advanced functional material development. Herein, we present the successful hydrothermal synthesis of tetragonal $CsPb_2Cl_5$ and the anion-exchange phase formation of $CsPb_2(Cl_{1-x}Br_x)_5$ (x = 0-1) solid solutions. The $CsPb_2(Cl_{1-x}Br_x)_5$ crystal structures, which crystallize in the tetragonal system, space group 14/mcm, with parameters similar to those of $CsPb_2Cl_5$, have been determined by Rietveld analysis. The optical band gap was obtained by UV-vis spectroscopy, and the band structure was further calculated by the full-potential method within the generalized gradient approximation. It was revealed that the band gap in $CsPb_2(Cl_{1-x}Br_x)_5$ solid solutions can be tuned over the range of 4.5-3.8 eV by anion substitution.

Accession Number: WOS:000441477100094
PubMed ID: 30010332
Author Identifiers:

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ISSN: 0020-1669
eISSN: 1520-510X

Record 76 of 214

Title: Highly accurate equilibrium structure of the C2h symmetric N1-to-O2 hydrogen-bonded uracil-dimer

Author(s): Kruse, H (Kruse, Holger); Sponer, J (Sponer, Jiri)

Source: INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **Volume:** 118 **Issue:** 15 **Article Number:** e25624 **DOI:** 10.1002/qua.25624 **Published:** AUG 5 2018

Abstract: The highly accurate ab initio equilibrium geometry of the hydrogen-bonded uracil dimer is derived using a composite geometry extrapolation scheme based on all-electron, complete basis set extrapolated MOller-Plesset perturbation theory using the jun-pwCV[T,Q]Z basis sets combined with a valence CCSD(T)/cc-pVTZ high-level correction. Geometrical changes on dimerization are discussed and the performance of the several density functional approximations (among others SCAN, B97M-V, DSD-PBEP86-D3(BJ), and DSD-PBEP86-NL) is evaluated. Orbital-optimized MP2.5 is discussed as a reduced-cost alternative to the CCSD(T) gradient in the composite scheme. A new reference interaction energy is calculated with explicitly correlated F12-CCSD(T).

Accession Number: WOS:000438343200018

Author Identifiers:

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Kruse, Holger	D-3615-2009	0000-0002-0560-1513

Record 77 of 214

Title: Anodic Deposition of Enantiopure Hexahelicene Layers

Author(s): Vacek, J (Vacek, Jan); Hrbac, J (Hrbac, Jan); Strasak, T (Strasak, Tomas); Cirkva, V (Cirkva, Vladimir); Sykora, J (Sykora, Jan); Fekete, L (Fekete, Ladislav); Pokorny, J (Pokorny, Jan); Bulir, J (Bulir, Jiri); Hromadova, M (Hromadova, Magdalena); Crassous, J (Crassous, Jeanne); Storch, J (Storch, Jan)

Source: CHEMELECTROCHEM **Volume:** 5 **Issue:** 15 **Pages:** 2080-2088 **DOI:** 10.1002/celc.201800565 **Published:** AUG 1 2018

Abstract: Helicenes are polyaromatic compounds with chiral properties useful for many applications in optoelectronics, separation processes, chiral recognition and catalysis. Here we focused on the electrochemistry of carbo[n]helicenes (n=5,6,7). The cyclic voltammograms of racemic mixtures of target compounds in acetonitrile/0.1M tetrabutylammonium perchlorate at a glassy carbon electrode reveal the diffusion-controlled reactions in both anodic and cathodic potential regions. Electrochemical behaviors are different for individual helicenes, [7]helicene undergoes redox transformation easily in comparison to the other investigated compounds, which is in agreement with DFT (density functional theory) calculations. Generally, the multi-component anodic process of helicenes is observable at potentials from +1.5 to +2.5V, leading to the formation of deposited structures (layers) on the electrode surface. The helicenes were electrodeposited onto transparent indium tin oxide (ITO) electrodes and characterized by atomic force microscopy, UV/Vis, Raman spectroscopy and ellipsometry. Finally, the anodic deposition of P and M enantiomers of [6]helicene was performed using ITO substrates, resulting in the formation of enantiopure layers of nanometer thicknesses, as confirmed by circular dichroism spectroscopy. The discovered electrosynthetic procedure opens up a new possibility for the immobilization of chiral helicene layers onto solid supports.

Accession Number: WOS:000440546600006

Author Identifiers:

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Fekete, Ladislav	F-7498-2011	0000-0002-8548-2613
Pokorny, Jan	F-4569-2011	0000-0002-2614-1667

Record 78 of 214

Title: Electric field determination in air plasmas from intensity ratio of nitrogen spectral bands: II. Reduction of the uncertainty and state-of-the-art model

Author(s): Bilek, P (Bilek, Petr); Obrusnik, A (Obrusnik, Adam); Hoder, T (Hoder, Tomas); Simek, M (Simek, Milan); Bonaventura, Z (Bonaventura, Zdenek)

Source: PLASMA SOURCES SCIENCE & TECHNOLOGY **Volume:** 27 **Issue:** 8 **Article Number:** 085012 **DOI:** 10.1088/1361-6595/aad666 **Published:** AUG 2018

Abstract: An established and widely used method for remote electric field determination is based on the ratio of the spectral band intensities of the first negative and second positive spectral systems of molecular nitrogen which does, however, require theoretically or experimentally obtained dependence R(E/N). The aim of this work is to reduce the overall uncertainty in the theoretical dependence R(E/N) calculated in part I of this work. We present an in-depth review of the kinetic and cross section data that are available in literature for the most influential processes. By tracking the historical evolution of the kinetic data, their cross-validation by independent authors and by taking into account advances in the experimental methods, we separate datasets that have not been rendered inaccurate by later works. By doing so, we reduce the uncertainty of the theoretical R(E/N) dependence and propose corresponding confidence band to be used by scientific community.

Accession Number: WOS:000443257000004

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Record 79 of 214

Title: Electric field determination in air plasmas from intensity ratio of nitrogen spectral bands: I. Sensitivity analysis and uncertainty quantification of dominant processes

Author(s): Obrusnik, A (Obrusnik, Adam); Bilek, P (Bilek, Petr); Hoder, T (Hoder, Tomas); Simek, M (Simek, Milan); Bonaventura, Z (Bonaventura, Zdenek)

Source: PLASMA SOURCES SCIENCE & TECHNOLOGY **Volume:** 27 **Issue:** 8 **Article Number:** 085013 **DOI:** 10.1088/1361-6595/aad663 **Published:** AUG 2018

Abstract: The ratio of the spectral band intensities of the first negative and second positive spectral systems of molecular nitrogen is a well recognized method for indirect determination of the electric field. It is applied for various plasmas, e.g. barrier and corona discharges for industrial applications or geophysical plasmas occurring in the Earth's atmosphere. The method relies on the dependence of the intensity ratio R(E/N) of selected bands on the reduced electric field strength. Both experimental and theoretical approaches have been used to determine this dependence, yet there is still a rather large spread in the data available in literature. The primary aim of this work is to quantify the overall uncertainty of the theoretical R(E/N) dependence and identify the main sources of this uncertainty. As the first step we perform sensitivity analysis on a full N-2/O-2 plasma kinetics model to find a minimal set of processes that are influential for the R(E/N) dependence. It is found to be in agreement with simplified kinetic models generally used. Subsequently, we utilize Monte Carlo-based uncertainty quantification to provide a confidence band for the electric field obtained from the theoretical R(E/N) dependence. Finally, subsequent steps are proposed to significantly reduce the uncertainty of the method.

Accession Number: WOS:000443257000005

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Record 80 of 214

Title: Characterization of the canine immunoglobulin heavy chain repertoire by next generation sequencing

Author(s): Hwang, MH (Hwang, Mei-Hua); Darzentas, N (Darzentas, Nikos); Bienzle, D (Bienzle, Dorothee); Moore, PF (Moore, Peter F.); Morrison, J (Morrison, Jodi); Keller, SM (Keller, Stefan M.)

Source: VETERINARY IMMUNOLOGY AND IMMUNOPATHOLOGY **Volume:** 202 **Pages:** 181-190 **DOI:** 10.1016/j.vetimm.2018.07.002 **Published:** AUG 2018

Abstract: The ability to mount adaptive immune responses to a diverse array of pathogens is essential to maintaining the health of an individual. The outcome of adaptive immune responses is influenced by the pool of available lymphocyte antigen receptors. Understanding the composition and dynamics of immune repertoires is hence of relevance to characterizing physiologic immunological processes as well as understanding disease pathogenesis. The dog is increasingly recognized as a model for human disease. The objective of this study was to utilize NGS for comprehensive and unbiased analysis of the IGH repertoire in healthy dogs. First, the IGH locus was searched in silico for previously unidentified genes. Second, IGH transcripts from major lymphoid organs were amplified using a 5'RACE approach without V/J primer bias. Third, amplicons were sequenced on an Illumine MiSeq platform, and data were analyzed using the ARResT/Interrogate platform. Data analysis included V/J usage, V-J pairing biases, isotype frequency, CDR3 diversity, convergent recombination, and public repertoires. The results of this study provide a comprehensive IGH repertoire analysis for healthy dogs. These data will allow further improvement of V/J gene-specific primer sets and will serve as baseline for future studies investigating immune repertoires in health and disease.

Accession Number: WOS:000442189700024

PubMed ID: 30078594

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ISSN: 0165-2427
eISSN: 1873-2534

Record 81 of 214
Title: USNO-B1.0 1452-0049820 and ASAS J102556+2049.3: Two W UMa Binaries Close to the Lower Mass-ratio Limit
Author(s): Kjurkchieva, DP (Kjurkchieva, Diana P.); Popov, VA (Popov, Velimir A.); Petrov, NI (Petrov, Nikola I.)
Source: ASTRONOMICAL JOURNAL **Volume:** 156 **Issue:** 2 **DOI:** 10.3847/1538-3881/aace5e **Published:** AUG 2018
Abstract: Photometric observations of the W UMa binaries USNO-Bl.O 1452-0049820 and ASAS J102556+2049.3 are presented. The results from the light curve solutions are as follows: (i) the component temperatures are T-1= 6400K and T-2 = 6300 K for USNO-Bl.O 1452-0049820 and T-1 = 6000 K and T-2 = 5930 K for ASAS J102556+2049; (ii) the photometric mass ratios are well determined because the targets undergo total eclipses; (iii) both mass ratios are close to the lower mass-ratio limit (0.111 and 0.131 correspondingly); (iv) the fillout factors of the two targets are unexpectedly small (0.045 and 0.243, respectively) for their mass ratios. The global parameters of the target components were estimated on the basis of the empirical relationship "period-total mass" for low mass-ratio binaries. We established a period decrease for ASAS J102556+2049.3 of dP/dt= -3.39 x lO(-6)day yr(-1).
Accession Number: WOS:000440747500001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
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ISSN: 0004-6256
eISSN: 1538-3881

Record 82 of 214
Title: Host subspecific viral strains in European house mice: Murine cytomegalovirus in the Eastern (Mus musculus musculus) and Western house mouse (Mus musculus domesticus)
Author(s): Cizkova, D (Cizkova, Dagmar); Baird, SJE (Baird, Stuart J. E.); Tesikova, J (Tesikova, Jana); Voigt, S (Voigt, Sebastian); Dureje, L (Dureje, Ludovit); Pialek, J (Pialek, Jaroslav); de Bellocq, JG (de Bellocq, Joelle Gouy)
Source: VIROLOGY **Volume:** 521 **Pages:** 92-98 **DOI:** 10.1016/j.virol.2018.05.023 **Published:** AUG 2018
Abstract: Murine cytomegalovirus (MCMV) has been reported from house mice (Mus musculus) worldwide, but only recently from Eastern house mice (M. m. musculus), of particular interest because they form a semi-permeable species barrier in Europe with Western house mice, M. in. domesticus. Here we report genome sequences of EastMCMV (from Eastern mice), and set these in the context of MCMV genomes from genus Mus hosts. We show EastMCMV and WestMCMV are genetically distinct. Phylogeny splitting analyses show a genome wide (94%) pattern consistent with no West-East introgression, the major exception (3.8%) being a genome-terminal region of duplicated genes involved in host immune system evasion. As expected from its function, this is a region of maintenance of ancestral polymorphism: The lack of clear splitting signal cannot be interpreted as evidence of introgression. The EastMCMV genome sequences reported here can therefore serve as a well-described resource for exploration of murid MCMV diversity.
Accession Number: WOS:000439956400010
PubMed ID: 29894896
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Dureje, Ludovit	F-9726-2014	
Gouy de Bellocq, Joelle	J-4733-2013	0000-0001-5831-6284
Pialek, Jaroslav	B-1237-2008	
Baird, Stuart	B-3872-2011	
Voigt, Sebastian		0000-0003-1544-9903

ISSN: 0042-6822

Record 83 of 214
Title: Stability of a behavioural syndrome vs. plasticity in individual behaviours over the breeding cycle: Ultimate and proximate explanations
Author(s): Trnka, A (Trnka, Alfred); Samas, P (Samas, Peter); Grim, T (Grim, Tomas)
Source: BEHAVIOURAL PROCESSES **Volume:** 153 **Pages:** 100-106 **DOI:** 10.1016/j.beproc.2018.06.003 **Published:** AUG 2018
Abstract: Animals often show correlated suites of consistent behavioural traits, i.e., personality or behavioural syndromes. Does this conflict with potential phenotypic plasticity which should be adaptive for animals facing various contexts and situations? This fundamental question has been tested predominantly in studies which were done in non-breeding contexts and under laboratory conditions. Therefore, in the present study we examined the temporal stability of behavioural correlations in a breeding context and under natural conditions. We found that in the great reed warbler (Acrocephalus arundinaceus) females, the intensity of their nest defence formed a behavioural syndrome with two other traits: their aggression during handling (self-defence) and stress responses during handling (breath rate). This syndrome was stable across the nesting cycle: each of the three behavioural traits was highly statistically repeatable between egg and nestling stages and the traits were strongly correlated with each other during both the egg stage and the nestling stage. Despite this consistency (i.e., rank order between stages) the individual behaviours changed their absolute values significantly during the same period. This shows that stable behavioural syndromes might be based on behaviours that are themselves unstable. Thus, syndromes do not inevitably constrain phenotypic plasticity. We suggest that the observed behavioural syndrome is the product of interactions between behavioural and life history trade-offs and that crucial proximate mechanisms for the plasticity and correlations between individual behaviours are hormonally-regulated.
Accession Number: WOS:000438833700013
PubMed ID: 29870797
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Samas, Peter	E-3152-2016	
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ISSN: 0376-6357
eISSN: 1872-8308

Record 84 of 214
Title: YANG/NETCONF ROADM: Evolving Open DWDM Toward SDN Applications
Author(s): Kundrat, J (Kundrat, Jan); Vojtech, J (Vojtech, Josef); Skoda, P (Skoda, Pavel); Vohnout, R (Vohnout, Rudolf); Radil, J (Radil, Jan); Havlis, O (Havlis, Ondrej)
Source: JOURNAL OF LIGHTWAVE TECHNOLOGY **Volume:** 36 **Issue:** 15 **Special Issue:** SI **Pages:** 3105-3114 **DOI:** 10.1109/JLT.2018.2822268 **Published:** AUG 1 2018
Abstract: Evolution in the field of optical networking in National Research and Education Networks led to utilization of Alien Wavelengths (AWs) and disaggregated Open Line Systems. Dynamic provisioning of AWs, in general spectrum services, is achieved via Reconfigurable Optical Add Drop Multiplexers (ROADMs) operating with flexible spectrum allocation. Northbound interface of these is usually implemented via the NETCONF protocol and through an appropriate Yet Another Next Generation (YANG) model. This paper presents a self-contained flexible spectral grid YANG model for low-level control and monitoring of a ROADM. The presented YANG model offers access to all functional components of a modern flexgrid ROADM and enables SDN applications to access and manipulate the media layer with no required external validation. The model is verified by an SDN application which implements optical path protection of AWs. A physical demonstration with model railroad intuitively shows the accomplished functionality.
Accession Number: WOS:000436536400006
Author Identifiers:

Author	ResearcherID Number	ORCID Number
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ISSN: 0733-8724
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Record 85 of 214

Title: Electronic, bonding, linear, and nonlinear optical properties of Na(2)MGe(2)Q(6) (M = Cd, Zn, Hg; Q = S, Se), Na2ZnSi2S6, and Na2ZnSn2S6 two metal-mixed chalcogenide compounds: Insights from an ab initio study

Author(s): Mahiaoui, R (Mahiaoui, R.); Ouahrani, T (Ouahrani, T.); Chikhaoui, A (Chikhaoui, A.); Morales-Garcia, A (Morales-Garcia, A.); Reshak, AH (Reshak, A. H.)

Source: JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS **Volume:** 119 **Pages:** 220-227 **DOI:** 10.1016/j.jpcs.2018.04.003 **Published:** AUG 2018

Abstract: In this study, in order to understand the origins of the bonding, electronic, and optical properties of Na(2)MGe(2)Q(6) (M = Cd, Zn, Hg; Q = S, Se), Na2ZnSi2S6, and Na2ZnSn2S6 compounds, we conducted first principles calculations within the density functional theory framework. We analyzed the sensitivity of replacing cations and anions with different electronegativity, which were rationalized in terms of the electronic structure and the contributions of different orbitals. Our calculations yielded lattice parameters, band gap, dipole moments, and second harmonic components that generally agreed well with the available experimental data. In addition, the electron localization function and atom-in-molecule topological formalisms were used to obtain further insights into the bonding properties. The calculations demonstrated the good concordance between the nature of the analyzed electronic domains and the response to second harmonic generation for the compounds studied. Moreover, the optical properties of these materials were found to be highly sensitive to the combined effects of the [Si/Ge/SnQ(4)] and [MQ(4)] units.

Accession Number: WOS:000432765100027

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ISSN: 0022-3697
eISSN: 1879-2553

Record 86 of 214

Title: Study of purinosome assembly in cell-based model systems with de novo purine synthesis and salvage pathway deficiencies

Author(s): Baresova, V (Baresova, Veronika); Skopova, V (Skopova, Vaclava); Souckova, O (Souckova, Olga); Krijt, M (Krijt, Matyas); Kmoch, S (Kmoch, Stanislav); Zikanova, M (Zikanova, Marie)

Source: PLOS ONE **Volume:** 13 **Issue:** 7 **Article Number:** e0201432 **DOI:** 10.1371/journal.pone.0201432 **Published:** JUL 30 2018

Abstract: Background
The enzymes involved in de novo purine synthesis (DNPS), one of the basic processes in eukaryotic cells, transiently and reversibly form a dynamic multienzyme complex called the purinosome in the cytoplasm. The purinosome has been observed in a broad spectrum of cells, but some studies claim that it is an artefact of the constructs used for visualization or stress granules resulting from the exposure of cells to nutrient-reduced growth media. Both may be true depending on the method of observation. To clarify this point, we combined two previously used methods, transfection and immunofluorescence, to detect purinosomes in purinosome-free cells deficient in particular DNPS steps (CR-DNPS cells) and in cells deficient in the salvage pathway, which resulted in construction of the purinosome regardless of purine level (CR-HGPRT cells).
Methods and findings
To restore or disrupt purinosome formation, we transiently transfected CR-DNPS and CR-HGPRT cells with vectors encoding BFP-labelled wild-type (wt) proteins and observed the normalization of purinosome formation. The cells also ceased to accumulate the substrate (s) of the defective enzyme. The CR-DNPS cell line transfected with a DNA plasmid encoding an enzyme with zero activity served as a negative control for purinosome formation. No purinosome formation was observed in these cells regardless of the purine level in the growth medium.
Conclusion
In conclusion, both methods are useful for the detection of purinosomes in HeLa cells. Moreover, the cell-based models prepared represent a unique system for the study of purinosome assembly with deficiencies in DNPS or in the salvage pathway as well as for the study of purinosome formation under the action of DNPS inhibitors. This approach is a promising step toward the treatment of purine disorders and can also provide targets for anticancer therapy.

Accession Number: WOS:000440251600041

PubMed ID: 30059557

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ISSN: 1932-6203

Record 87 of 214

Title: A novel combined experimental and multiscale theoretical approach to unravel the structure of SiC/SiOx core/shell nanowires for their optimal design

Author(s): Morresi, T (Morresi, Tommaso); Timpel, M (Timpel, Melanie); Pedrielli, A (Pedrielli, Andrea); Garberoglio, G (Garberoglio, Giovanni); Tatti, R (Tatti, Roberta); Verucchi, R (Verucchi, Roberto); Pasquali, L (Pasquali, Luca); Pugno, NM (Pugno, Nicola Maria); Nardi, MV (Nardi, Marco Vittorio); Taioli, S (Taioli, Simone)

Source: NANOSCALE **Volume:** 10 **Issue:** 28 **Pages:** 13449-13461 **DOI:** 10.1039/c8nr03712d **Published:** JUL 28 2018

Abstract: In this work we propose a realistic model of nanometer-thick SiC/SiOx core/shell nanowires (NWs) using a combined first-principles and experimental approach. SiC/SiOx core/shell NWs were first synthesised by a low-cost carbothermal method and their chemical-physical experimental analysis was accomplished by recording X-ray absorption near-edge spectra. In particular, the K-edge absorption lineshapes of C, O, and Si are used to validate our computational model of the SiC/SiOx core/shell NW architectures, obtained by a multiscale approach, including molecular dynamics, tight-binding and density functional simulations. Moreover, we present ab initio calculations of the electronic structure of hydrogenated SiC and SiC/SiOx core/shell NWs, studying the modification induced by several different substitutional defects and impurities into both the surface and the interfacial region between the SiC core and the SiOx shell. We find that on the one hand the electron quantum confinement results in a broadening of the band gap, while hydroxyl surface terminations decrease it. This computational investigation shows that our model of SiC/SiOx core/shell NWs is capable to deliver an accurate interpretation of the recorded X-ray absorption near-edge spectra and proves to be a valuable tool towards the optimal design and application of these nanosystems in actual devices.

Accession Number: WOS:000439319000019

PubMed ID: 29972180

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Record 88 of 214

Title: An intricate balance of hydrogen bonding, ion atmosphere and dynamics facilitates a seamless uracil to cytosine substitution in the U-turn of the neomycin-sensing riboswitch

Author(s): Krepl, M (Krepl, Miroslav); Vogele, J (Voegele, Jennifer); Kruse, H (Kruse, Holger); Duchardt-Ferner, E (Duchardt-Ferner, Elke); Wohnert, J (Woehnert, Jens); Sponer, J (Sponer, Jiri)

Source: NUCLEIC ACIDS RESEARCH **Volume:** 46 **Issue:** 13 **Pages:** 6528-6543 **DOI:** 10.1093/nar/gky490 **Published:** JUL 27 2018

Abstract: The neomycin sensing riboswitch is the smallest biologically functional RNA riboswitch, forming a hairpin capped with a U-turn loop-a well-known RNA motif containing a conserved uracil. It was shown previously that a U -> C substitution of the eponymous conserved uracil does not alter the riboswitch structure due to C protonation at N3. Furthermore, cytosine is evolutionary permitted to replace uracil in other U-turns. Here, we use molecular dynamics simulations to study the molecular basis of this substitution in the neomycin sensing riboswitch and show that a structure-stabilizing monovalent cation-binding site in the wild-type RNA is the main reason for its negligible structural effect. We then use NMR spectroscopy to confirm the existence of this cation-binding site and to demonstrate its effects on RNA stability. Lastly, using quantum chemical calculations, we show that the cation-binding site is altering the electronic environment of the wild-type U-turn so that it is more similar to the cytosine mutant. The study reveals an amazingly complex and delicate interplay between various energy contributions shaping up the 3D structure and evolution of nucleic acids.

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PubMed ID: 29893898

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Record 89 of 214

Title: Efficient Strategy for Determining the Atomic-Resolution Structure of Micro- and Nanocrystalline Solids within Polymeric Microbeads: Domain-Edited NMR Crystallography

Author(s): Brus, J (Brus, Jiri); Czernek, J (Czernek, Jiri); Hruby, M (Hruby, Martin); Svec, P (Svec, Pavel); Kobera, L (Kobera, Libor); Abbrent, S (Abbrent, Sabina); Urbanova, M (Urbanova, Martina)

Source: MACROMOLECULES   **Volume:** 51   **Issue:** 14   **Pages:** 5364-5374   **DOI:** 10.1021/acs.macromol.8b00392   **Published:** JUL 24 2018

Abstract: Precise structural analysis of multiphase polymeric nanocomposites remains a challenge even in the presence of high quality X-ray diffraction data. This contribution thus addresses our attempt to formulate a combined analytical strategy for obtaining the atomic-resolution structure of multicomponent polymeric solids with complex nanodomain architecture. In this strategy, through the application of T-1-filtered solid-state NMR spectroscopy, the individual components are successively distinguished and selected, and the corresponding H-1, C-13, and N-15 isotropic chemical shifts are explicitly assigned. Thereafter, using an automated protocol allowing for processing and statistical analysis of large data sets, the experimentally determined NMR parameters are systematically compared with those DFT-calculated for the representative set of crystal structure predictions. Particular attention is devoted to the analysis of NMR parameters of hydrogen-bonded protons which are responsible for molecular packing. As a result of this search, the structures of micro- and nanosized crystallites dispersed in the polymeric matrix are determined and independently verified by the measurements of through-space dipolar couplings. The potential of this strategy is demonstrated on injectable polyanhydride microbeads consisting of a mixture of microcrystalline decitabine and nanocrystalline sebacic acid, both incorporated in the semicrystalline polymeric matrix of poly(sebacic acid). Through the synergistic interplay between the measurements, calculations, and the statistical analysis, we have developed an integrated approach providing structural information that is challenging to elucidate using conventional diffraction approaches. This combination of experimental and theoretical approaches enables one to determine the structural arrangements of molecules in situations which are not tractable by conventional spectroscopic techniques.

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Record 90 of 214

Title: Conformational changes allow processing of bulky substrates by a haloalkane dehalogenase with a small and buried active site

Author(s): Kokkonen, P (Kokkonen, Piia); Bednar, D (Bednar, David); Dockalova, V (Dockalova, Veronika); Prokop, Z (Prokop, Zbynek); Damborsky, J (Damborsky, Jiri)

Source: JOURNAL OF BIOLOGICAL CHEMISTRY   **Volume:** 293   **Issue:** 29   **Pages:** 11505-11512   **DOI:** 10.1074/jbc.RA117.000328   **Published:** JUL 20 2018

Abstract: Haloalkane dehalogenases catalyze the hydrolysis of halogen-carbon bonds in organic halogenated compounds and as such are of great utility as biocatalysts. The crystal structures of the haloalkane dehalogenase DhlA from the bacterium from Xanthobacter autotrophicus GJ10, specifically adapted for the conversion of the small 1,2-dichloroethane (DCE) molecule, display the smallest catalytic site (110 angstrom(3)) within this enzyme family. However, during a substrate-specificity screening, we noted that DhlA can catalyze the conversion of far bulkier substrates, such as the 4-(bromomethyl)-6,7-dimethoxy-coumarin (220 angstrom(3)). This large substrate cannot bind to DhlA without conformational alterations. These conformational changes have been previously inferred from kinetic analysis, but their structural basis has not been understood. Using molecular dynamic simulations, we demonstrate here the intrinsic flexibility of part of the cap domain that allows DhlA to accommodate bulky substrates. The simulations displayed two routes for transport of substrates to the active site, one of which requires the conformational change and is likely the route for bulky substrates. These results provide insights into the structure-dynamics function relationships in enzymes with deeply buried active sites. Moreover, understanding the structural basis for the molecular adaptation of DhlA to 1,2-dichloroethane introduced into the biosphere during the industrial revolution provides a valuable lesson in enzyme design by nature.

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PubMed ID: 29858243

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ISSN: 0021-9258
eISSN: 1083-351X

Record 91 of 214

Title: Implementing efficient concerted rotations using Mathematica and C code

Author(s): Tubiana, L (Tubiana, Luca); Jurasek, M (Jurasek, Miroslav); Coluzza, I (Coluzza, Ivan)

Source: EUROPEAN PHYSICAL JOURNAL E   **Volume:** 41   **Issue:** 7   **Article Number:** 87   **DOI:** 10.1140/epje/i2018-11694-7   **Published:** JUL 20 2018

Abstract: In this article we demonstrate a general and efficient metaprogramming implementation of concerted rotations using Mathematica. Concerted rotations allow the movement of a fixed portion of a polymer backbone with fixed bending angles, like a protein, while maintaining the correct geometry of the backbone and the initial and final points of the portion fixed. Our implementation uses Mathematica to generate a C code which is then wrapped in a library by a Python script. The user can modify the Mathematica notebook to generate a set of concerted rotations suited for a particular backbone geometry, without having to write the C code himself. The resulting code is highly optimized, performing on the order of thousands of operations per second.

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eISSN: 1292-895X

Record 92 of 214

Title: Magic-Angle Spinning Frequencies beyond 300 kHz Are Necessary To Yield Maximum Sensitivity in Selectively Methyl Protonated Protein Samples in Solid-State NMR

Author(s): Xue, K (Xue, Kai); Sarkar, R (Sarkar, Riddhiman); Motz, C (Motz, Carina); Asami, S (Asami, Sam); Decker, V (Decker, Venita); Wegner, S (Wegner, Sebastian); Tosner, Z (Tosner, Zdenek); Reif, B (Reif, Bernd)

Source: JOURNAL OF PHYSICAL CHEMISTRY C   **Volume:** 122   **Issue:** 28   **Pages:** 16437-16442   **DOI:** 10.1021/acs.jpcc.8b05600   **Published:** JUL 19 2018

Abstract: In the last decade, proton detection in magic-angle spinning (MAS) solid-state NMR became a popular strategy for biomolecular structure determination. In particular, probe technology has experienced tremendous progress with smaller and smaller diameter rotors achieving ever higher MAS frequencies. MAS rotation frequencies beyond 100 kHz allow to observe and assign protons in fully protonated samples. In these experiments, resolution is however compromised as homogeneous proton-proton dipolar coupling interactions are not completely averaged out. Using a combination of experiments and simulations, we analyze the MAS frequency dependent intensities of the H-1,C-13 methyl correlation peaks of a selectively methyl protonated (CH3) microcrystalline sample of the chicken a-spectrin SH3 domain (alpha-SH3). Extensive simulations involving nine spins employing the program SIMPSON allow to predict the MAS frequency dependence of the proton intensities. The experimental results are used to validate the simulations. As quantitative measure, we determine the characteristic MAS frequency, which is necessary to obtain >50% of the maximum achievable sensitivity. Our results show that this frequency is site-specific and strongly depends on the local methyl density. We find that the characteristic MAS frequency ranges from as low as 20 kHz up to 324 kHz with the average value of 135 +/- 88 kHz for this particular sample at a magnetic field strength of 11.7 T. Inclusion of side chain dynamics in the analysis reduces the average characteristic MAS frequency to 104 +/- 68 kHz within the range of 11-261 kHz. In case, >80% of the maximum sensitivity shall be achieved, MAS rotation frequencies of 498 +/- 370 and 310 +/- 227 kHz are required with and without including side chains dynamics in the analysis, respectively.

Record 93 of 214

Title: In Situ Formation of N-Heterocyclic Carbene-Bound Single-Molecule Junctions

Author(s): Doud, EA (Doud, Evan A.); Inkpen, MS (Inkpen, Michael S.); Lovat, G (Lovat, Giacomo); Montes, E (Montes, Enrique); Paley, DW (Paley, Daniel W.); Steigerwald, ML (Steigerwald, Michael L.); Vazquez, H (Vazquez, Hector); Venkataraman, L (Venkataraman, Latha); Roy, X (Roy, Xavier)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 140 **Issue:** 28 **Pages:** 8944-8949 **DOI:** 10.1021/jacs.8b05184 **Published:** JUL 18 2018

Abstract: Self-assembled monolayers (SAMs) formed using N-heterocyclic carbenes (NHCs) have recently emerged as thermally and chemically ultrastable alternatives to those formed from thiols. The rich chemistry and strong sigma-donating ability of NHCs offer unique prospects for applications in nanoelectronics, sensing, and electrochemistry. Although stable in SAMs, free carbenes are notoriously reactive, making their electronic characterization challenging. Here we report the first investigation of electron transport across single NHC-bound molecules using the scanning tunneling microscope-based break junction (STM-BJ) technique. We develop a series of air-stable metal NHC complexes that can be electrochemically reduced in situ to form NHC electrode contacts, enabling reliable single molecule conductance measurements of NHCs under ambient conditions. Using this approach, we show that the conductance of an NHC depends on the identity of the single metal atom to which it is coordinated in the junction. Our observations are supported by density functional theory (DFT) calculations, which also firmly establish the contributions of the NHC linker to the junction transport characteristics. Our work demonstrates a powerful method to probe electron transfer across NHC electrode interfaces; more generally, it opens the door to the exploitation of surface-bound NHCs in constructing novel, functionalized electrodes and/or nanoelectronic devices.

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Record 94 of 214

Title: Reactivity of orthophthalaldehyde with aliphatic, alicyclic and aromatic primary diamines: Electrochemical study and mechanistic considerations

Author(s): Dazie, JD (Dazie, Joel Donkeng); Liska, A (Liska, Alan); Urban, J (Urban, Jiri); Ludvik, J (Ludvik, Jiri)

Source: JOURNAL OF ELECTROANALYTICAL CHEMISTRY **Volume:** 821 **Special Issue:** SI **Pages:** 131-139 **DOI:** 10.1016/j.jelechem.2018.02.019 **Published:** JUL 15 2018

Abstract: The reactions of OPA with eight primary diamines were electrochemically monitored and the main products were isolated and identified. Various types of diamines were used: two non-vicinal alpha,omega-diaminoalkanes, four vicinal 1,2-diamino(cyclo)alkanes and two aromatic diamines. The results showed three electrochemical patterns: a,to aliphatic diamines and both aromatic diamines exhibited only consumption of the parent OPA without observation of any electroactive intermediate or product; aliphatic and alicyclic vicinal diamines react with OPA under fast formation of reducible intermediate and its slow follow-up reaction yielding reducible product. A special case represents 1,2-trans-diaminocyclohexane exhibiting different products with regard to its cis-isomer. The main reaction products in all cases are derivatives of indano[1,2-a]benzimidazole and not bis-Schiff bases discussed in the literature.
It has been found that the reaction of non-vicinal diamines with OPA is much faster than that of the vicinal diamines. The UV vis monitoring revealed that the reaction of OPA with vicinal, as well as non-vicinal diamines results in the same type of product, hence the mentioned difference in the electrochemical pattern is caused by different kinetics. The slower reaction rate can be caused by lower nucleophilicity of vicinal diamines, where stronger electronic communication of vicinal amino groups takes place. This effect manifests itself as larger difference between the first and second pKa of the two amine groups and the comparison of HOMOs supported this interpretation.

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Record 95 of 214

Title: Genomic Prediction in a Multiploid Crop: Genotype by Environment Interaction and Allele Dosage Effects on Predictive Ability in Banana

Author(s): Nyine, M (Nyine, Moses); Uwimana, B (Uwimana, Brigitte); Blavet, N (Blavet, Nicolas); Hribova, E (Hribova, Eva); Vanrespaille, H (Vanrespaille, Helena); Batte, M (Batte, Michael); Akech, V (Akech, Violet); Brown, A (Brown, Allan); Lorenzen, J (Lorenzen, Jim); Swennen, R (Swennen, Rony); Dolezel, J (Dolezel, Jaroslav)

Source: PLANT GENOME **Volume:** 11 **Issue:** 2 **Article Number:** UNSP 170090 **DOI:** 10.3835/plantgenome2017.10.0090 **Published:** JUL 2018

Abstract: Improving the efficiency of selection in conventional crossbreeding is a major priority in banana (Musa spp.) breeding. Routine application of classical marker assisted selection (MAS) is lagging in banana due to limitations in MAS tools. Genomic selection (GS) based on genomic prediction models can address some limitations of classical MAS, but the use of GS in banana has not been reported to date. The aim of this study was to evaluate the predictive ability of six genomic prediction models for 15 traits in a multi-ploidy training population. The population consisted of 307 banana genotypes phenotyped under low and high input field management conditions for two crop cycles. The single nucleotide polymorphism (SNP) markers used to fit the models were obtained from genotyping by sequencing (GBS) data. Models that account for additive genetic effects provided better predictions with 12 out of 15 traits. The performance of BayesB model was superior to other models particularly on fruit filling and fruit bunch traits. Models that included averaged environment data were more robust in trait prediction even with a reduced number of markers. Accounting for allele dosage in SNP markers (AD-SNP) reduced predictive ability relative to traditional biallelic SNP (BA-SNP), but the prediction trend remained the same across traits. The high predictive values (0.47-0.75) of fruit filling and fruit bunch traits show the potential of genomic prediction to increase selection efficiency in banana breeding.

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Record 96 of 214

Title: Role of Inosine-Uracil Base Pairs in the Canonical RNA Duplexes

Author(s): Spackova, N (Spackova, Nad'a); Reblova, K (Reblova, Kamila)

Source: GENES **Volume:** 9 **Issue:** 7 **Article Number:** 324 **DOI:** 10.3390/genes9070324 **Published:** JUL 2018

Abstract: Adenosine to inosine (A-I) editing is the most common modification of double-stranded RNA (dsRNA). This change is mediated by adenosine deaminases acting on RNA (ADARs) enzymes with a preference of U>A>C>G for 5' neighbor and G>C=A>U or G>C>U=A for 3' neighbor. A-I editing occurs most frequently in the non-coding regions containing repetitive elements such as ALUs. It leads to disruption of RNA duplex structure, which prevents induction of innate immune response. We employed standard and biased molecular dynamics (MD) simulations to analyze the behavior of RNA duplexes with single and tandem inosine-uracil (I-U) base pairs in different sequence context. Our analysis showed that the I-U pairs induce changes in base pair and base pair step parameters and have different dynamics when compared with standard canonical base pairs. In particular, the first I-U pair from tandem I-U/I-U systems exhibited increased dynamics depending on its neighboring 5' base. We discovered that UII sequence, which is frequently edited, has lower flexibility compared with other sequences (AII, GII, CII), hence it only modestly disrupts dsRNA. This might indicate that the UAA motifs in ALUs do not have to be sufficiently effective in preventing immune signaling.

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ISSN: 2073-4425

Record 97 of 214
Title: Dynamics and interactions of membrane-anchored cytochromes P450
Author(s): Jerabek, P (Jerabek, P.); Florian, J (Florian, J.); Martinek, V (Martinek, V.)
Source: FEBS OPEN BIO **Meeting Abstract:** S.44-3 **Volume:** 8 **Pages:** 20-20 **Supplement:** 1 **Published:** JUL 2018
Accession Number: WOS:000437674100049
ISSN: 2211-5463

Record 98 of 214
Title: Membrane-bound cytochrome P450s of 1A subfamily features similar structural pattern of the trans-membrane segment
Author(s): Jerabek, P (Jerabek, P.); Florian, J (Florian, J.); Martinek, V (Martinek, V.)
Source: FEBS OPEN BIO **Meeting Abstract:** P.11-016-M **Volume:** 8 **Pages:** 352-353 **Supplement:** 1 **Published:** JUL 2018
Accession Number: WOS:000437674104130
ISSN: 2211-5463

Record 99 of 214
Title: Structure of supercooled water: Polarizable BK3 model versus non-polarizable models
Author(s): Skvara, J (Skvara, Jiri); Moucka, F (Moucka, Filip); Nezbeda, I (Nezbeda, Ivo)
Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 261 **Pages:** 303-318 **DOI:** 10.1016/j.molliq.2018.03.117 **Published:** JUL 1 2018
Abstract: The polarizable BK3 model of water was simulated, using both Monte Carlo and molecular dynamics methods, along isobars p = 1 and 1000 bar for temperatures ranging from supercritical down to 228.15 K with the focus on details of its structure and changes with temperature. Since overwhelming majority of results for supercooled model water have been obtained for non-polarizable models, in most cases the ST2 one, we also simulated at corresponding conditions this model along with another, and qualitatively different non-polarizable model, TIP4P/Ice for comparison. In addition to commonly used various order parameters to characterize the structure, and a detailed analysis of the spatial distribution function over the first three coordination shells, we also employ a geometric construction based on the Delaunay tessellation, the method independent of any a priori defined quantity. All these analyses aim at an examination to what extent qualitative differences in the models (force fields) affect the observed structure. It is found that in most cases the polarizable BK3 model and TIP4P/Ice water yield very similar structural properties. On the contrary, ST2 water exhibits, in majority cases, even qualitatively different properties and these findings are discussed in detail. The obtained results suggest that any conclusion on the behavior of supercooled water based on the ST2 model should be taken, at least, with caution. (C) 2018 Elsevier B.V. All rights reserved.
Accession Number: WOS:000436222000032
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Record 100 of 214
Title: Structural Stability of Peptidic His-Containing Proton Wire in Solution and in the Adsorbed State
Author(s): Dorcak, V (Dorcak, Vlastimil); Novak, D (Novak, David); Kabelac, M (Kabelac, Martin); Kroutil, O (Kroutil, Ondrej); Bednarova, L (Bednarova, Lucie); Veverka, V (Veverka, Vaclav); Vacek, J (Vacek, Jan)
Source: LANGMUIR **Volume:** 34 **Issue:** 24 **Pages:** 6997-7005 **DOI:** 10.1021/acs.langmuir.7b04139 **Published:** JUN 19 2018
Abstract: Molecular wires are functional molecules applicable in the field of transfer processes in technological and biochemical applications. Besides molecular wires with the ability to transfer electrons, research is currently focused on molecular wires with high proton affinity and proton transfer ability. Recently, proposed peptidic proton wires (H wires) are one example. Their ability to mediate the transport of protons from aqueous solutions onto the surface of a Hg electrode in a catalytic hydrogen evolution reaction was investigated by constant-current chronopotentiometric stripping. However, elucidating the structure of H wires and rationalizing their stability are key requirements for their further research and application. In this article, we focus on the His (H) and Ala (A)-containing peptidic H wire A(3)-(H-A(2))(6) in solution and after its immobilization onto the electrode surface in the presence of the secondary structure stabilizer 2,2,2-trifluoroethanol (TFE). We found that the solvent containing more than 25% of TFE stabilizes the helical structure of A(3)-(H-A(2))(6) not only in solution but also in the adsorbed state. The TFE efficacy to stabilize alpha-helical structure was confirmed using high-resolution nuclear magnetic resonance, circular dichroism, and molecular dynamics simulation. Experimental and theoretical results indicated A3-(H-A(2))(6) to be a high proton-affinity peptidic H wire with an alpha-helical structure stabilized by TFE, which was confirmed in a comparative study with hexahistidine as an example of a peptide with a definitely disordered and random coil structure. The results presented here could be used for further investigation of the peptidic H wires and for the application of electrochemical methods in the research of proton transfer phenomena in general.
Accession Number: WOS:000436022900003
PubMed ID: 29763545
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Record 101 of 214

Title: The Nature of Chemical Bonding in Lewis Adducts as Reflected by Al-27 NMR Quadrupolar Coupling Constant: Combined Solid-State NMR and Quantum Chemical Approach

Author(s): Kobera, L (Kobera, Libor); Czernek, J (Czernek, Jiri); Abbrent, S (Abbrent, Sabina); Mackova, H (Mackova, Hana); Pavlovec, L (Pavlovec, Lukas); Rohlicek, J (Rohlicek, Jan); Brus, J (Brus, Jiri)

Source: INORGANIC CHEMISTRY **Volume:** 57 **Issue:** 12 **Pages:** 7428-7437 **DOI:** 10.1021/acs.inorgchem.8b01009 **Published:** JUN 18 2018

Abstract: Lewis acids and Lewis adducts are widely used in the chemical industry because of their high catalytic activity. Their precise geometrical description and understanding of their electronic structure are a crucial step for targeted synthesis and specific use. Herein, we present an experimental/computational strategy based on a solidstate NMR crystallographic approach allowing for detailed structural characterization of a wide range of organoaluminum compounds considerably differing in their chemical constitution. In particular, we focus on the precise measurement and subsequent quantumchemical analysis of many different Al-27 NMR resonances in the extremely broad range of quadrupolar coupling constants from 1 to 50 MHz. In this regard, we have optimized an experimental strategy combining a range of static as well as magic angle spinning experiments allowing reliable detection of the entire set of aluminum sites present in trimesitylaluminum (AlMes(3)) reaction products. In this way, we have spectroscopically resolved six different products in the resulting polycrystalline mixture. All Al-27 NMR resonances are precisely recorded and comprehensively analyzed by a quantum-chemical approach. Interestingly, in some cases the recorded Al-27 solid-state NMR spectra show unexpected quadrupolar coupling constant values reaching up to ca. 30 MHz, which are attributed to tetra-coordinated aluminum species (Lewis adducts with trigonal pyramidal geometry). The cause of this unusual behavior is explored by analyzing the natural bond orbitals and complexation energies. The linear correlation between the quadrupolar coupling constant value and the nature of bonds in the Lewis adducts is revealed. Moreover, the Al-27 NMR data are shown to be sensitive to the geometry of the tetra-coordinated organoaluminum species. Our findings thus provide a viable approach for the direct identification of Lewis acids and Lewis adducts, not only in the investigated multicomponent organoaluminum compounds but also in inorganic zeolites featuring catalytically active trigonal (Al-III) and strongly perturbed Al-IV sites.

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Pavlovec, Lukas	D-4919-2016	
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Record 102 of 214

Title: Binding of Lanthanide Complexes to Histidine-Containing Peptides Probed by Raman Optical Activity Spectroscopy

Author(s): Brichtova, E (Brichtova, Eva); Hudecova, J (Hudecova, Jana); Vrskova, N (Vrskova, Nikola); Sebestik, J (Sebestik, Jaroslav); Bour, P (Bour, Petr); Wu, T (Wu, Tao)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 24 **Issue:** 34 **Pages:** 8664-8669 **DOI:** 10.1002/chem.201800840 **Published:** JUN 18 2018

Abstract: Lanthanide complexes are used as convenient spectroscopic probes for many biomolecules. Their binding to proteins is believed to be enhanced by the presence of histidine, but the strength of the interaction significantly varies across different systems. To understand the role of peptide length and sequence, short histidine-containing peptides have been synthesized (His-Gly, His-Gly-Gly, His-Gly-Gly-Gly, Gly-His, Gly-His-Gly, His-His, and Gly-Gly-His) and circularly polarized luminescence (CPL) induced at the [Eu(dpa)(3)](3-) complex has been measured by means of a Raman optical activity (ROA) spectrometer. The obtained data indicate relatively weak binding of the histidine residue to the complex, with a strong participation of other parts of the peptide. Longer peptides, low pH, and a histidine residue close to the N-peptide terminus favor the binding. The binding strengths are approximately proportional to the CPL intensity and roughly correlate with predictions based on molecular dynamics (MD) simulations. The specificity of lanthanide binding to the peptide structure and its intense luminescence and high optical activity make the ROA/CPL technique suitable for probing secondary and tertiary structures of peptides and proteins.

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ISSN: 0947-6539

eISSN: 1521-3765

Record 103 of 214

Title: EasyMiner.eu: Web framework for interpretable machine learning based on rules and frequent itemsets

Author(s): Vojir, S (Vojir, Stanislav); Zeman, V (Zeman, Vaclav); Kuchar, J (Kuchar, Jaroslav); Kliegr, T (Kliegr, Tomas)

Source: KNOWLEDGE-BASED SYSTEMS **Volume:** 150 **Pages:** 111-115 **DOI:** 10.1016/j.knosys.2018.03.006 **Published:** JUN 15 2018

Abstract: EasyMiner (http://www.easyminer.eu) is a web-based system for interpretable machine learning based on frequent itemsets. It currently offers association rule learning (apriori, FP-Growth) and classification (CBA). EasyMiner offers a visual interface designed for interactivity, allowing the user to define a constraining pattern for the mining task. The CBA algorithm can also be used for pruning of the rule set, thus addressing the common problem of "too many rules" on the output, and the implementation supports automatic tuning of confidence and support thresholds. The development version additionally supports anomaly detection (FPI and its variations) and linked data mining (AMIE+). EasyMiner is dockerized, some of its components are available as open source R packages. (C) 2018 Elsevier B.V. All rights reserved.

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Record 104 of 214

Title: Chemical potentials of alkaline earth metal halide aqueous electrolytes and solubility of their hydrates by molecular simulation: Application to CaCl2, antarcticite, and sinjarite

Author(s): Moucka, F (Moucka, Filip); Kolafa, J (Kolafa, Jiri); Lisal, M (Lisal, Martin); Smith, WR (Smith, William R.)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 148 **Issue:** 22 **Article Number:** 222832 **DOI:** 10.1063/1.5024212 **Published:** JUN 14 2018

Abstract: We present a molecular-level simulation study of CaCl2 in water and crystalline hydrates formed by CaCl2 at ambient (298.15 K, 1 bar) conditions and at a high-temperature high-pressure state (365 K, 275 bars) typical of hydraulic fracturing conditions in natural-gas extraction, at which experimental properties are poorly characterized. We focus on simulations of chemical potentials in both solution and crystalline phases and on the salt solubility, the first time to our knowledge that such properties have been investigated by molecular simulation for divalent aqueous electrolytes. We first extend our osmotic ensemble Monte Carlo simulation technique [F. Mou. cka et al., J. Phys. Chem. B 115, 7849-7861 (2011)] to such solutions. We then describe and apply newmethodology for the simulation of the chemical potentials of the experimentally observed crystalline hydrates at ambient conditions (antarcticite, CaCl2 center dot 6H(2)O) and at high-temperature conditions (sinjarite, CaCl2 center dot 2H(2)O). We implement our methodologies using for both phases the CaCl2 transferable force field (FF) based on simple point charge-extended water developed by Mamatkulov et al. [J. Chem. Phys. 138, 024505 (2013)], based on training sets involving single-ion and ion-pair low-concentration solution properties at near-ambient conditions. We find that simulations of the solution chemical potentials at high concentrations are somewhat problematic, exhibiting densities diverging from experimental values and accompanied by dramatically decreasing particle mobility. For the solid phases, the sinjarite crystalline lattice differs from experiment only slightly, whereas the simulations of antarcticite completely fail, due to instability of the crystalline lattice. The FF thus only successfully yields the sinjarite solubility, but its value m = 8.0(7) mol kg(-1) H2O lies well below the experimentally observed solubility range at 1 bar pressure of (12m, 15m) in the temperature interval (320 K, 400 K). We conclude that the used FF does not provide a good description of the experimental properties considered and suggest that improvement must take into account the crystalline properties. Published by AIP Publishing.

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Title: Description and Comparative Genomics of Macrococcus caseolyticus subsp hominis subsp nov., Macrococcus goetzii sp nov., Macrococcus epidermidis sp nov., and Macrococcus bohemicus sp nov., Novel Macrococci From Human Clinical Material With Virulence Potential and Suspected Uptake of Foreign DNA by Natural Transformation

Author(s): Maslanova, I (Maslanova, Ivana); Wertheimer, Z (Wertheimer, Zuzana); Sedlacek, I (Sedlacek, Ivo); Svec, P (Svec, Pavel); Indrakova, A (Indrakova, Adela); Kovarovic, V (Kovarovic, Vojtech); Schumann, P (Schumann, Peter); Sproer, C (Sproeer, Cathrin); Kralova, S (Kralova, Stanislava); Sedo, O (Sedo, Ondrej); Kristofova, L (Kristofova, Lucie); Vrbovska, V (Vrbovska, Veronika); Fuzik, T (Fuzik, Tibor); Petras, P (Petras, Petr); Zdrahal, Z (Zdrahal, Zbynek); Ruzickova, V (Ruzickova, Vladislava); Doskar, J (Doskar, Jiri); Pantucek, R (Pantucek, Roman)

Abstract: The genus Macrococcus is a close relative of the genus Staphylococcus. Whilst staphylococci are widespread as human pathogens, macrococci have not yet been reported from human clinical specimens. Here we investigated Gram-positive and catalase-positive cocci recovered from human clinical material and identified as Macrococcus sp. by a polyphasic taxonomic approach and by comparative genomics. Relevant phenotypic, genotypic and chemotaxonomic methods divided the analyzed strains into two separate clusters within the genus Macrococcus. Comparative genomics of four representative strains revealed enormous genome structural plasticity among the studied isolates. We hypothesize that high genomic variability is due to the presence of a com operon, which plays a key role in the natural transformation of bacilli and streptococci. The possible uptake of exogenous DNA by macrococci can contribute to a different mechanism of evolution from staphylococci, where phage-mediated horizontal gene transfer predominates. The described macrococcal genomes harbor novel plasmids, genomic islands and islets, as well as prophages. Capsule gene clusters, intracellular protease, and a fibronectin-binding protein enabling opportunistic pathogenesis were found in all four strains. Furthermore, the presence of a CRISPR-Cas system with 90 spacers in one of the sequenced genomes corresponds with the need to limit the burden of foreign DNA. The highly dynamic genomes could serve as a platform for the exchange of virulence and resistance factors, as was described for the methicillin resistance gene, which was found on the novel composite SCCmec-like element containing a unique mec gene complex that is considered to be one of the missing links in SCC evolution. The phenotypic, genotypic, chemotaxonomic and genomic results demonstrated that the analyzed strains represent one novel subspecies and three novel species of the genus Macrococcus, for which the names Macrococcus caseolyticus subsp. hominis subsp. nov. (type strain CCM 7927(T) = DSM 103682(T)), Macrococcus goetzii sp. nov. (type strain CCM 4927(T) = DSM 103683(T)), Macrococcus epidermidis sp. nov. (type strain CCM 7099(T) = DSM 103681(T)), and Macrococcus bohemicus sp. nov. (type strain CCM 7100(T) = DSM 103680(T)) are proposed. Moreover, a formal description of Macrococcus caseolyticus subsp. caseolyticus subsp. nov. and an emended description of the genus Macrococcus are provided.

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Title: Electronic structure and magnetic anisotropies of antiferromagnetic transition-metal difluorides

Author(s): Correa, CA (Correa, Cinthia Antunes); Vyborny, K (Vyborny, Karel)

Abstract: We compare calculations based on density functional theory (DFT) with available experimental data and analyze the origin of magnetic anisotropies in MnF_2, FeF_2, CoF_2, and NiF_2. We confirm that the magnetic anisotropy of MnF_2 stems almost completely from the dipolar interaction, while magnetocrystalline anisotropy energy (originating in spin-orbit interaction) plays a dominant role in the other three compounds, and discuss how it depends on the details of band structure. The latter is critically compared to available optical measurements. The case of CoF_2, where magnetocrystalline anisotropy energy strongly depends on U (the Hubbard parameter in DFT+U), is put into contrast with FeF_2 where theoretical predictions of magnetic anisotropies are nearly quantitative.

Title: Origin of Vibrational Instabilities in Molecular Wires with Separated Electronic States

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

Abstract: Current-induced heating in molecular junctions stems from the interaction between tunneling electrons and localized molecular vibrations. If the electronic excitation of a given vibrational mode exceeds heat dissipation, a situation known as vibrational instability is established, which can seriously compromise the integrity of the junction. Using out of equilibrium first-principles calculations, we demonstrate that vibrational instabilities can take place in the general case of molecular wires with separated unoccupied electronic states. From the ab initio results, we derive a model to characterize unstable vibrational modes and construct a diagram that maps mode stability. These results generalize previous theoretical work and predict vibrational instabilities in a new regime.

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Title: Red Clover (Trifolium pratense) and Zigzag Clover (T-medium) - A Picture of Genomic Similarities and Differences

Author(s): Dluhosova, J (Dluhosova, Jana); Istvanek, J (Istvanek, Jan); Nedelnik, J (Nedelnik, Jan); Repkova, J (Repkova, Jana)

Abstract: The genus clover (Trifolium sp.) is one of the most economically important genera in the Fabaceae family. More than 10 species are grown as manure plants or forage legumes. Red clover's (T. pratense) genome size is one of the smallest in the Trifolium genus, while many clovers with potential breeding value have much larger genomes. Zigzag clover (T. medium) is closely related to the sequenced red clover; however, its genome is approximately 7.5x larger. Currently, almost nothing is known about the architecture of this large genome and differences between these two clover species. We sequenced the T. medium genome (2n = 8x = 64) with similar to 23x coverage and managed to partially assemble 492.7 Mbp of its genomic sequence. A thorough comparison between red clover and zigzag clover sequencing reads resulted in the successful validation of 7 T. pratense-and 45 T. medium-specific repetitive elements. The newly discovered repeats led to the set-up of the first partial T. medium karyotype. Newly discovered red clover and zigzag clover tandem repeats were summarized. The structure of centromere-specific satellite repeat resembling that of T. repens was inferred in T. pratense. Two repeats, TrM300 and TrM378, showed a specific localization into centromeres of a half of all zigzag clover chromosomes; TrM300 on eight chromosomes and TrM378 on 24 chromosomes. A comparison with the red clover draft sequence was also used to mine more than 105,000 simple sequence repeats (SSRs) and 1,170,000 single nucleotide variants (SNVs). The presented data obtained from the sequencing of zigzag clover represent the first glimpse on the genomic sequence of this species. Centromeric repeats indicated its allopolyploid origin and naturally occurring homogenization of the centromeric repeat motif was somehow prevented. Using various repeats, highly uniform 64 chromosomes were separated into eight types of chromosomes. Zigzag clover genome underwent substantial chromosome rearrangements and cannot be counted as a true octoploid. The resulting data, especially the large number of predicted SSRs and SNVs, may have great potential for further research of the legume family and for rapid advancements in clover breeding.

Record 109 of 214
Title: Two-dimensional modeling of density and thermal structure of dense circumstellar outflowing disks

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

Abstract: Context. Evolution of massive stars is affected by a significant loss of mass either via (nearly) spherically symmetric stellar winds or by aspherical mass-loss mechanisms, namely the outflowing equatorial disks. However, the scenario that leads to the formation of a disk or rings of gas and dust around massive stars is still under debate. It is also unclear how various forming physical mechanisms of the circumstellar environment affect its shape and density, as well as its kinematic and thermal structure.
Aims. We study the hydrodynamic and thermal structure of optically thick, dense parts of outflowing circumstellar disks that may be formed around various types of critically rotating massive stars, for example, Be stars, B[e] supergiant (sgB[e]) stars or Pop III stars. We calculate self-consistent time-dependent models of temperature and density structure in the disk's inner dense region that is strongly affected by irradiation from a rotationally oblate central star and by viscous heating.
Methods. Using the method of short characteristics, we specify the optical depth of the disk along the line-of-sight from stellar poles. Within the optically thick dense region with an optical depth of tau > 2 = 3 we calculate the vertical disk thermal structure using the diffusion approximation while for the optically thin outer layers we assume a local thermodynamic equilibrium with the impinging stellar irradiation. For time-dependent hydrodynamic modeling, we use two of our own types of hydrodynamic codes: two-dimensional operator-split numerical code based on an explicit Eulerian finite volume scheme on a staggered grid, and unsplit code based on the Roe's method, both including full second-order Navier-Stokes shear viscosity.
Results. Our models show the geometric distribution and contribution of viscous heating that begins to dominate in the central part of the disk for mass-loss rates higher than (M) over dot greater than or similar to 10(-10) M-circle dot yr(-1). In the models of dense viscous disks with (M) over dot > 10(-8) M-circle dot yr(-1), the viscosity increases the central temperature up to several tens of thousands of Kelvins, however the temperature rapidly drops with radius and with distance from the disk midplane. The high mass-loss rates and high viscosity lead to instabilities with significant waves or bumps in density and temperature in the very inner disk region.
Conclusions. The two-dimensional radial-vertical models of dense outflowing disks including the full Navier-Stokes viscosity terms show very high temperatures that are however limited to only the central disk cores inside the optically thick area, while near the edge of the optically thick region the temperature may be low enough for the existence of neutral hydrogen, for example.

Record 110 of 214
Title: Gene expression profiling in healthy newborns from diverse localities of the Czech Republic

Author(s): Honkova, K (Honkova, Katerina); Rossnerova, A (Rossnerova, Andrea); Pavlikova, J (Pavlikova, Jitka); Svecova, V (Svecova, Vlasta); Klema, J (Klema, Jiri); Topinka, J (Topinka, Jan); Milcova, A (Milcova, Alena); Libalova, H (Libalova, Helena); Choi, H (Choi, Hyunok); Veleminsky, M (Veleminsky, Milos); Sram, RJ (Sram, Radim J.); Rossner, P (Rossner, Pavel, Jr.)

Abstract: Prenatal exposure to air pollution is associated with intrauterine growth restriction and low birth weight. Gene expression changes in newborns in relation to air pollution have not been sufficiently studied. We analyzed whole genome expression in cord blood leukocytes of 202 newborns from diverse localities of the Czech Republic, differing among other factors in levels of air pollution: the district of Karvina (characterized by higher concentration of air pollutants) and Ceske Budejovice (lower air pollution levels). We aimed to identify differentially expressed genes (DEGs) and pathways in relation to locality and concentration of air pollutants. We applied the linear model to identify the specific DEGs and the correlation analysis, to investigate the relationship between the concentrations of air pollutants and gene expression data. An analysis of biochemical pathways and gene set enrichment was also performed. In general, we observed modest changes of gene expression, mostly attributed to the effect of the locality. The highest number of DEGs was found in samples from the district of Karvina. A pathway analysis revealed a deregulation of processes associated with cell growth, apoptosis or cellular homeostasis, immune response-related processes or oxidative stress response. The association between concentrations of air pollutants and gene expression changes was weak, particularly for samples collected in Karvina. In summary, as we did not find a direct effect of exposure to air pollutants, we assume that the general differences in the environment, rather than actual concentrations of individual pollutants, represent a key factor affecting gene expression changes at delivery. Environ. Mol. Mutagen. 59:401-415, 2018. (c) 2018 Wiley Periodicals, Inc.

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Record 111 of 214
Title: Determining the Crystal Structures of Peptide Analogs of Boronic Acid in the Absence of Single Crystals: Intricate Motifs of Ixazomib Citrate Revealed by XRPD Guided by ss-NMR

Author(s): Husak, M (Husak, Michal); Jegorov, A (Jegorov, Alexandr); Rohlicek, J (Rohlicek, Jan); Fitch, A (Fitch, Andrew); Czernek, J (Czernek, Jiri); Kobera, L (Kobera, Libor); Brus, J (Brus, Jiri)

Abstract: Uncertainties in the structure determination of peptide analogs of boronic acid, exacerbated by the many coordination modes of boron, represent an obstacle in understanding their role in living organisms and thus also in developing the next generation of anticancer drugs. For that reason, we present here a general experimental computational strategy allowing structure determination of complex boronic acid derivatives with extensive conformational variability. We demonstrate successful solution of the crystal structures of two nonsolvated polymorphs of ixazomib citrate directly from synchrotron powder diffraction data, which is challenging because the two molecules in the asymmetric unit cell that exhibit 32 degrees of conformational freedom push the limits of current solution procedures. We used a novel two-step Rietveld refinement based on DFT-D restraints to improve information quality derived from powder diffraction data to be comparable with that of single crystal solutions. NMR crystallography was applied to verify the crystal structures, and the high potential value of using B-11 NMR parameters toward the solution of unknown structures was demonstrated. Evolution of B-11-B-11 double-quantum coherences allows probing of interatomic distances up to 7 angstrom. Overall, we present an integrated approach that applies several techniques in conjunction to provide otherwise unavailable structural information.

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Record 112 of 214
Title: Relativistic Spin-Orbit Heavy Atom on the Light Atom NMR Chemical Shifts: General Trends Across the Periodic Table Explained

Author(s): Vicha, J (Vicha, Jan); Komorovsky, S (Komorovsky, Stanislav); Repisky, M (Repisky, Michal); Marek, R (Marek, Radek); Straka, M (Straka, Michal)

Abstract: The importance of relativistic effects on the NMR parameters in heavy-atom (HA) compounds, particularly the SO-HALA (Spin-Orbit Heavy Atom on the Light Atom) effect on NMR chemical shifts, has been known for about 40 years. Yet, a general correlation between the electronic structure and SO-HALA effect has been missing. By analyzing H-1 NMR chemical shifts of the sixth-period hydrides (Cs-At), we discovered general electronic-structure principles and mechanisms that dictate the size and sign of the SO-HALA NMR chemical shifts. In brief, partially occupied HA valence shells induce relativistic shielding at the light atom (LA) nuclei, while empty HA valence shells induce relativistic deshielding. In particular, the LA nucleus is relativistically shielded in 5d(2)-5d(8) and 6p(4) HA hydrides and deshielded in 4f(0), 5d(0), 6s(0), and 6p(0) HA hydrides. This general and intuitive concept explains periodic trends in the H-1 NMR chemical shifts along the sixth-period hydrides (Cs-At) studied in this work. We present substantial evidence that the introduced principles have a general validity across the periodic table and can be extended to nonhydride LAs. The decades-old question of why compounds with occupied frontier pi molecular orbitals (MOs) cause SO-HALA shielding at the LA nuclei, while the frontier sigma MOs cause deshielding is answered. We further derive connection between the SO-HALA NMR chemical shifts and

Spin-Orbit-induced Electron Deformation Density (SO-EDD), a property that can be obtained easily from differential electron densities and can be represented graphically. SO-EDD provides an intuitive understanding of the SO-HALA effect in terms of the depletion/concentration of the electron density at LA nuclei caused by spin-orbit coupling due to HA in the presence of a magnetic field. Using an analogy between the SO-EDD concept and arguments from classic NMR theory, the complex question of the SO-HALA NMR chemical shifts becomes easily understandable for a wide chemical audience.

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Title: An ant genus-group (Prenolepis) illuminates the biogeography and drivers of insect diversification in the Indo-Pacific

Author(s): Matos-Maravi, P (Matos-Maravi, Pavel); Clouse, RM (Clouse, Ronald M.); Sarnat, EM (Sarnat, Eli M.); Economo, EP (Economo, Evan P.); LaPolla, JS (LaPolla, John S.); Borovanska, M (Borovanska, Michaela); Rabeling, C (Rabeling, Christian); Czekanski-Moir, J (Czekanski-Moir, Jesse); Latumahina, F (Latumahina, Fransina); Wilson, EO (Wilson, Edward O.); Janda, M (Janda, Milan)

Source: MOLECULAR PHYLOGENETICS AND EVOLUTION **Volume:** 123 **Pages:** 16-25 **DOI:** 10.1016/j.ympev.2018.02.007 **Published:** JUN 2018

Abstract: The Malay Archipelago and the tropical South Pacific (hereafter the Indo-Pacific region) are considered biodiversity hotspots, yet a general understanding of the origins and diversification of species-rich groups in the region remains elusive. We aimed to test hypotheses for the evolutionary processes driving insect species diversity in the Indo-Pacific using a higher-level and comprehensive phylogenetic hypothesis for an ant clade consisting of seven genera. We estimated divergence times and reconstructed the biogeographical history of ant species in the Prenolepis genus-group (Formicidae: Formicinae: Lasiini). We used a fossil-calibrated phylogeny to infer ancestral geographical ranges utilizing a biogeographic model that includes founder-event speciation. Ancestral state reconstructions of the ants' ecological preferences, and diversification rates were estimated for selected Indo-Pacific clades. Overall, we report that faunal interchange between Asia and Australia has occurred since at least 20-25 Ma, and early dispersal to the Fijian Basin happened during the early and mid-Miocene (ca. 10-20 Ma). Differences in diversification rates across Indo-Pacific clades may be related to ecological preference breadth, which in turn may have facilitated geographical range expansions. Ancient dispersal routes suggested by our results agree with the palaeogeography of the region. For this particular group of ants, the rapid orogenesis in New Guinea and possibly subsequent ecological shifts may have promoted their rapid diversification and widespread distribution across the Indo-Pacific.

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Title: Development of polymorphic microsatellites for the invasive Asian fish tapeworm Schyzocotyle acheilognathi

Author(s): Brabec, J (Brabec, Jan); Scholz, T (Scholz, Tomas); Stefka, J (Stefka, Jan)

Source: PARASITOLOGY INTERNATIONAL **Volume:** 67 **Issue:** 3 **Pages:** 341-343 **DOI:** 10.1016/j.parint.2018.01.007 **Published:** JUN 2018

Abstract: We describe the development of ready-to-use set of fifteen polymorphic microsatellite markers to benefit future population biology and phylogeographic studies on the invasive Asian fish tapeworm Schyzocotyle acheilognathi. The microsatellite loci were selected from partial Illumina shotgun genome sequences of three parasite specimens and their universality tested on a set of 12 geographically distant populations of the parasite. Particularly low levels of heterozygosity have been detected in the Chinese population pointing towards possible hidden population structure that deserves further attention in future population genetic studies.

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Title: Mechanical and thermal properties of graphene random nanofoams via Molecular Dynamics simulations

Author(s): Pedrielli, A (Pedrielli, Andrea); Taioli, S (Taioli, Simone); Garberoglio, G (Garberoglio, Giovanni); Pugno, NM (Pugno, Nicola Maria)

Source: CARBON **Volume:** 132 **Pages:** 766-775 **DOI:** 10.1016/j.carbon.2018.02.081 **Published:** JUN 2018

Abstract: Graphene foams have recently attracted a great deal of interest for their possible use in technological applications, such as electrochemical storage devices, wearable electronics, and chemical sensing. In this work, we present computational investigations, performed by using molecular dynamics with reactive potentials, of the mechanical and thermal properties of graphene random nanofoams. In particular, we assess the mechanical and thermal performances of four families of random foams characterized by increasing mass density and decreasing average pore size. We find that the foams' mechanical performances under tension cannot be rationalized in terms of mass density, while they are principally related to their topology. Under compression, higher-density foams show the typical slope change in the stress-strain curve at 5 - 10% strain, moving from linear elasticity to a buckling region. At variance, lower density foams display a quasi-linear behavior up to 35% strain. Furthermore, we assess the thermal conductivity of these random foams using the Green-Kubo approach. While foam thermal conductivity is affected by both connectivity and defects, nevertheless we obtain similar values for all the investigated families, which means that topology is the critical factor affecting thermal transport in these structures. (c) 2018 Elsevier Ltd. All rights reserved.

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Title: Rapid Water Transport through Organic Layers on Ice

Author(s): Kong, XR (Kong, Xiangrui); Toubin, C (Toubin, Celine); Habartova, A (Habartova, Alena); Pluharova, E (Pluharova, Eva); Roeselova, M (Roeselova, Martina); Pettersson, JBC (Pettersson, Jan B. C.)

Source: JOURNAL OF PHYSICAL CHEMISTRY A **Volume:** 122 **Issue:** 21 **Pages:** 4861-4868 **DOI:** 10.1021/acs.jpca.8b01951 **Published:** MAY 31 2018

Abstract: Processes involving atmospheric aerosol and cloud particles are affected by condensation of organic compounds that are omnipresent in the atmosphere. On ice particles, organic compounds with hydrophilic functional groups form hydrogen bonds with the ice and orient their hydrophobic groups away from the surface. The organic layer has been expected to constitute a barrier to gas uptake, but recent experimental studies suggest that the accommodation of water molecules on ice is only weakly affected by condensed short-chain alcohol layers. Here, we employ molecular dynamics simulations to study the water interactions with n-butanol covered ice at 200 K and show that the small effect of the condensed layer is due to efficient diffusion of water molecules along the surface plane while seeking appropriate sites to penetrate, followed by penetration driven by the combined

attractive forces from butanol OH groups and water molecules within the ice. The water molecules that penetrate through the n-butanol layer become strongly bonded by approximately three hydrogen bonds at the butanol ice interface. The obtained accommodation coefficient (0.81 +/- 0.03) is in excellent agreement with results from previous environmental molecular beam experiments, leading to a picture where an adsorbed n-butanol layer does not alter the apparent accommodation coefficient but dramatically changes the detailed molecular dynamics and kinetics.

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PubMed ID: 29741896

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ISSN: 1089-5639

Record 117 of 214

Title: Diquats with Robust Chirality: Facile Resolution, Synthesis of Chiral Dyes, and Application as Selectors in Chiral Analysis

Author(s): Talele, HR (Talele, Harish R.); Koval, D (Koval, Dusan); Severa, L (Severa, Lukas); Reyes-Gutierrez, PE (Reyes-Gutierrez, Paul E.); Cisarova, I (Cisarova, Ivana); Sazelova, P (Sazelova, Petra); Saman, D (Saman, David); Bednarova, L (Bednarova, Lucie); Kasicka, V (Kasicka, Vaclav); Teply, F (Teply, Filip)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 24 **Issue:** 30 **Pages:** 7601-7604 **DOI:** 10.1002/chem.201800369 **Published:** MAY 28 2018

Abstract: Diquats with extremely high racemization barriers with G(theor) of 233kJmol(-1) at 180 degrees C are described. Reported configurational robustness is due to a combination of two structural features: the rigid o-xylylene tether connecting the nitrogen atoms and the presence of two substituents in the bay region of the bipyridinium scaffold. The straightforward synthesis of diquats, plus facile resolution and derivatization make them attractive for chiral application studies. This is demonstrated by: 1)synthesis of the first non-racemic diquat dyes with pronounced chiroptical properties, and 2)capability of diquats to interact stereospecifically with chiral molecules. This suggests potential for diquat derivatives to be used as chiral selectors in separation methods.

Accession Number: WOS:000434089500006

PubMed ID: 29575285

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ISSN: 0947-6539

eISSN: 1521-3765

Record 118 of 214

Title: Ab initio prediction of the polymorph phase diagram for crystalline methanol

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

Source: CHEMICAL SCIENCE **Volume:** 9 **Issue:** 20 **Pages:** 4622-4629 **DOI:** 10.1039/c8sc01237g **Published:** MAY 28 2018

Abstract: Organic crystals frequently adopt multiple distinct polymorphs exhibiting different properties. The ability to predict not only what crystal forms might occur, but under what experimental thermodynamic conditions those polymorphs are stable would be immensely valuable to the pharmaceutical industry and others. Starting only from knowledge of the experimental crystal structures, this study successfully predicts the methanol crystal polymorph phase diagram from first-principles quantum chemistry, mapping out the thermodynamic regions of stability for three polymorphs over the range 0-400 K and 0-6 GPa. The agreement between the predicted and experimental phase diagrams corresponds to predicting the relative polymorph free energies to within approximate to 0.5 kJ mol(-1) accuracy, which is achieved by employing fragment-based second-order MOller-Plesset perturbation theory and coupled cluster theory plus a quasi-harmonic treatment of the phonons.

Accession Number: WOS:000433426700009

PubMed ID: 29899955

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ISSN: 2041-6520

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Record 119 of 214

Title: An ab initio study of mechanical and dynamical stability of MoSi2

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

Source: JOURNAL OF ALLOYS AND COMPOUNDS **Volume:** 746 **Pages:** 720-728 **DOI:** 10.1016/j.jallcom.2018.01.241 **Published:** MAY 25 2018

Abstract: We present a quantum-mechanical study of changes in the electronic structure, total energy, elastic properties, phonon spectra and structure of molybdenum disilicide (MoSi2) with tetragonal C11(b) structure due to uniaxial strains along the [001] direction, biaxial (epitaxial) loads within the (001) plane as well as triaxial (volumetric) strains/stresses. Total energies and optimized structural parameters are computed by the Vienna Ab initio Simulation Package (VASP) using the local density approximation (LDA). When simulating extreme loading conditions that may be relevant for highly-strained regions we predict a semi-metal to metal phase transition that is connected with the onset of mechanical instability for higher values of triaxial loads as well as many other multi-axial loading conditions. The instability is assessed by both rigorous Born-Huang's criteria connected with elastic stiffness coefficients as well by phonon spectra computed for all three straining modes. The values of theoretical tensile strength of MoSi2 for uniaxial, biaxial and triaxial loading corresponding to the first phonon instability amount to 30, 41 and 35 GPa, respectively. We show that the semi-metal to metal transition is connected with the softening of acoustic phonons at the G point rather than with the instability of other phonon modes. (C) 2018 Elsevier B.V. All rights reserved.

Accession Number: WOS:000429170300087

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ISSN: 0925-8388

eISSN: 1873-4669

Record 120 of 214

Title: Experimental and theoretical study on cation-pi interaction of the univalent silver cation with pyrene in the gas phase and in the solid state

Author(s): Klepetarova, B (Klepetarova, Blanka); Kvicalova, M (Kvicalova, Magdalena); Sykora, D (Sykora, David); Makrlik, E (Makrlik, Emanuel); Vanura, P (Vanura, Petr)

Source: INORGANICA CHIMICA ACTA **Volume:** 477 **Pages:** 165-171 **DOI:** 10.1016/j.ica.2018.03.029 **Published:** MAY 24 2018

Abstract: By means of electrospray ionization mass spectrometry (ESI-MS), it was evidenced experimentally that the univalent silver cation (Ag+) reacts with the electroneutral pyrene ligand (C16H10) to form especially the cationic complexes [Ag(C16H10)](+) and [Ag(C16H10)(2)](+). Moreover, applying quantum chemical calculations, five different conformations of these two Ag(I) complexes were derived. Finally, in the solid state, the polymeric complex structure [Ag(pyrene)(0.5)(CF3SO3)](n)center dot[Ag(toluene)(CF3SO3)](n), crystallizing in the monoclinic system with the centrosymmetric space group P2/c, was prepared and analyzed by X-ray crystallography. (C) 2018 Elsevier B.V. All rights reserved.

Accession Number: WOS:000429902200023

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Record 121 of 214

Title: Gallium substitution in the transuranium superconductor PuCoGa5

Author(s): Colineau, E (Colineau, E.); Boulet, P (Boulet, P.); Griveau, JC (Griveau, J. -C.); Eloirdi, R (Eloirdi, R.); Wastin, F (Wastin, F.); Shick, AB (Shick, A. B.); Caciuffo, R (Caciuffo, R.)

Source: JOURNAL OF ALLOYS AND COMPOUNDS **Volume:** 745 **Pages:** 477-482 **DOI:** 10.1016/j.jallcom.2018.02.116 **Published:** MAY 15 2018

Abstract: We have studied the effects of substituting gallium by aluminum, germanium, tin and indium in PuCoGa5, the actinide-based superconductor with the highest critical temperature. By annealing arc-melted samples, we have been able to synthesize only compounds with 20% substitution by Al and Ge (i.e. PuCoGa4Al and PuCoGa4Ge). Refinements of X-ray powder diffraction patterns for these two compounds indicate an enhanced c/a ratio, whereas magnetic susceptibility measurements reveal a large reduction of the critical temperature T-c compared to PuCoGa5. DFT+ED calculations indicate that the decrease of T-c is accompanied by significant changes in the Fermi surface. Finally, measurements on PuCoGa5 samples made by using Ga-69 and Ga-71 isotopes showed no effect of the atomic mass of gallium on the superconducting critical temperature. (C) 2018 Elsevier B.V. All rights reserved.

Accession Number: WOS:000429163800058

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Record 122 of 214

Title: Protein environment affects the water-tryptophan binding mode. MD, QM/MM, and NMR studies of engrailed homeodomain mutants

Author(s): Spackova, N (Spackova, Nad'a); Trosanova, Z (Trosanova, Zuzana); Sebesta, F (Sebesta, Filip); Jansen, S (Jansen, Severine); Burda, JV (Burda, Jaroslav V.); Srb, P (Srb, Pavel); Zachrdla, M (Zachrdla, Milan); Zidek, L (Zidek, Lukas); Kozelka, J (Kozelka, Jiri)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 20 **Issue:** 18 **Pages:** 12664-12677 **DOI:** 10.1039/c7cp08623g **Published:** MAY 14 2018

Abstract: Water molecules can interact with aromatic moieties using either their O-H bonds or their lone-pairs of electrons. In proteins, water-pi interactions have been reported to occur with tryptophan and histidine residues, and dynamic exchange between O-H center dot center dot center dot pi hydrogen bonding and lone-pair center dot center dot center dot pi interactions was suggested to take place, based on ab initio calculations. Here we used classical and QM/MM molecular dynamics simulations, complemented with an NMR study, to examine a specific water-indole interaction observed in the engrailed homeodomain and in its mutants. Our simulations indicate that the binding mode between water and indole can adapt to the potential created by the surrounding amino acids (and by the residues at the DNA surface in protein-DNA complexes), and support the model of dynamic switching between the O-H center dot center dot center dot pi hydrogen bonding and lone-pair center dot center dot center dot pi binding modes.

Accession Number: WOS:000431825300034

PubMed ID: 29696277

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ISSN: 1463-9076

eISSN: 1463-9084

Record 123 of 214

Title: Anisotropic Approach for Simulating Electron Transport in Layered Materials: Computational and Experimental Study of Highly Oriented Pyrolitic Graphite

Author(s): Azzolini, M (Azzolini, Martina); Morresi, T (Morresi, Tommaso); Abrams, K (Abrams, Kerry); Masters, R (Masters, Robert); Stehling, N (Stehling, Nicola); Rodenburg, C (Rodenburg, Cornelia); Pugno, NM (Pugno, Nicola M.); Taioli, S (Taioli, Simone); Dapor, M (Dapor, Maurizio)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 122 **Issue:** 18 **Pages:** 10159-10166 **DOI:** 10.1021/acs.jpcc.8b02256 **Published:** MAY 10 2018

Abstract: In this work, we propose a theoretical and computational model for taking into account the anisotropic structure of highly oriented pyrolitic graphite (HOPG) in the Monte Carlo simulations of charge transport. In particular, the dielectric characteristics, such as the inelastic mean free path and energy losses, are treated by linearly combining the contributions along the two main orthogonal directions identifying the layered crystalline structure of HOPG (along the layer plane and perpendicular to it). Energy losses are evaluated from ab initio calculations of the dielectric function of the system along these two perpendicular directions. Monte Carlo simulated spectra, obtained with our anisotropic approach, are compared with acquired experimental data of reflection electron energy loss and secondary electron spectra, showing a good agreement. These findings validate the idea of the importance of considering properly weighted interplanar and intraplanar interactions in the simulation of electron transport in layered materials.

Accession Number: WOS:000432477400047

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ISSN: 1932-7447

Record 124 of 214

Title: On Street-Canyon Flow Dynamics: Advanced Validation of LES by Time-Resolved PIV

Author(s): Kellnerova, R (Kellnerova, Radka); Fuka, V (Fuka, Vladimir); Uruba, V (Uruba, Vaclav); Jurcakova, K (Jurcakova, Klara); Nosek, S (Nosek, Stepan); Chaloupecka, H (Chaloupecka, Hana); Janour, Z (Janour, Zbynek)

Source: ATMOSPHERE **Volume:** 9 **Issue:** 5 **Article Number:** 161 **DOI:** 10.3390/atmos9050161 **Published:** MAY 2018

Abstract: The advanced statistical techniques for qualitative and quantitative validation of Large Eddy Simulation (LES) of turbulent flow within and above a two-dimensional street canyon are presented. Time-resolved data from 3D LES are compared with those obtained from time-resolved 2D Particle Image Velocimetry (PIV) measurements. We have extended a standard validation approach based solely on time-mean statistics by a novel approach based on analyses of the intermittent flow dynamics. While the standard Hit rate validation metric indicates not so good agreement between compared values of both the streamwise and vertical velocity within the canyon canopy, the Fourier, quadrant and Proper Orthogonal Decomposition (POD) analyses demonstrate very good LES prediction of highly energetic and characteristic features in the flow. Using the quadrant analysis, we demonstrated similarity between the model and the experiment with respect to the typical shape of intensive sweep and ejection events and their frequency of appearance. These findings indicate that although the mean values predicted by the LES do not meet the criteria of all the standard validation metrics, the dominant coherent structures are simulated well.

Accession Number: WOS:000435190300004

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ISSN: 2073-4433

Record 125 of 214

Title: Formation of chelate structure between His-Met dipeptide and diaqua-cisplatin complex; DFT/PCM computational study

Author(s): Maixner, M (Maixner, Michal); Dos Santos, HF (Dos Santos, Helio F.); Burda, JV (Burda, Jaroslav V.)

Source: JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY **Volume:** 23 **Issue:** 3 **Pages:** 363-376 **DOI:** 10.1007/s00775-018-1536-x **Published:** MAY 2018

Abstract: Interaction of cisplatin in activated diaqua-form with His-Met dipeptide is explored using DFT approach with PCM model. First the conformation space of the dipeptide is explored to find the most stable structure (labeled 0683). Several functionals with double-zeta basis set are used for optimization and obtained order of conformers is confirmed by the CCSD(T) single-point calculations. Supermolecular model is used to determine reaction coordinate for the replacement of aqua ligands consequently by N-site of histidine and S-site of methionine and reversely. Despite the monoadduct of Pt-S(Met) is thermodynamically less stable this reaction passes substantially faster (by several orders of magnitude) than coordination of cisplatin to histidine. The consequent chelate formation occurs relatively fast with energy release up to 12 kcal mol(-1).

Record 126 of 214
Title: Correlation effects in superconducting quantum dot systems
Author(s): Pokorny, V (Pokorny, Vladislav); Zonda, M (Zonda, Martin)
Source: PHYSICA B-CONDENSED MATTER **Volume:** 536 **Pages:** 488-491 **DOI:** 10.1016/j.physb.2017.08.059 **Published:** MAY 1 2018

Abstract: We study the effect of electron correlations on a system consisting of a single-level quantum dot with local Coulomb interaction attached to two superconducting leads. We use the single-impurity Anderson model with BCS superconducting baths to study the interplay between the proximity induced electron pairing and the local Coulomb interaction. We show how to solve the model using the continuous-time hybridization-expansion quantum Monte Carlo method. The results obtained for experimentally relevant parameters are compared with results of self-consistent second order perturbation theory as well as with the numerical renormalization group method.

Conference Title: International Conference on Strongly Correlated Electron Systems (SCES)
Conference Date: JUL 17-21, 2017
Conference Location: Prague, CZECH REPUBLIC
Conference Sponsors: Charles Univ, Fac Math & Phys, Dept Condensed Matter Phys
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Record 127 of 214
Title: Efficient sparse matrix-delayed vector multiplication for discretized neural field model
Author(s): Fousek, J (Fousek, Jan)
Source: JOURNAL OF SUPERCOMPUTING **Volume:** 74 **Issue:** 5 **Pages:** 1863-1884 **DOI:** 10.1007/s11227-017-2194-4 **Published:** MAY 2018

Abstract: Computational models of the human brain provide an important tool for studying the principles behind brain function and disease. To achieve whole-brain simulation, models are formulated at the level of neuronal populations as systems of delayed differential equations. In this paper, we show that the integration of large systems of sparsely connected neural masses is similar to well-studied sparse matrix-vector multiplication; however, due to delayed contributions, it differs in the data access pattern to the vectors. To improve data locality, we propose a combination of node reordering and tiled schedules derived from the connectivity matrix of the particular system, which allows performing multiple integration steps within a tile. We present two schedules: with a serial processing of the tiles and one allowing for parallel processing of the tiles. We evaluate the presented schedules showing speedup up to 2x on single-socket CPU, and 1.25x on Xeon Phi accelerator.

Author Identifiers:

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

Record 128 of 214
Title: Role of membrane cholesterol in differential sensitivity of muscarinic receptor subtypes to persistently bound xanomeline
Author(s): Randakova, A (Randakova, Alena); Dolejsi, E (Dolejsi, Eva); Rudajev, V (Rudajev, Vladimir); Zimcik, P (Zimcik, Pavel); Dolezal, V (Dolezal, Vladimir); El-Fakahany, EE (El-Fakahany, Esam E.); Jakubik, J (Jakubik, Jan)
Source: NEUROPHARMACOLOGY **Volume:** 133 **Pages:** 129-144 **DOI:** 10.1016/j.neuropharm.2018.01.027 **Published:** MAY 1 2018

Abstract: Xanomeline (3-(Hexyloxy)-4-(1-methy1-1,2,5,6-tetrahydropyridin-3-yl)-1,2,5-thiadiazole) is a muscarinic agonist that is considered to be functionally selective for the M-1/M-4 receptor subtypes. Part of xanomeline binding is resistant to washing. Wash-resistant xanomeline activates muscarinic receptors persistently, except for the M-5 subtype. Mutation of leucine 6.46 to isoleucine at M-1 or M-4 receptors abolished persistent activation by wash-resistant xanomeline. Reciprocal mutation of isoleucine 6.46 to leucine at the M-5 receptor made it sensitive to activation by wash-resistant xanomeline. Lowering of membrane cholesterol made M-1 and M-4 mutants and M-5 wild type receptors sensitive to activation by wash-resistant xanomeline. Molecular docking revealed a cholesterol binding site in the groove between transmembrane helices 6 and 7. Molecular dynamics showed that interaction of cholesterol with this binding site attenuates receptor activation. We hypothesize that differences in cholesterol binding to this site between muscarinic receptor subtypes may constitute the basis for xanomeline apparent functional selectivity and may have notable therapeutic implications. Differences in receptor-membrane interactions, rather than in agonist-receptor interactions, represent a novel possibility to achieve pharmacological selectivity. Our findings may be applicable to other G protein coupled receptors. (C) 2018 The Authors. Published by Elsevier Ltd.

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Record 129 of 214
Title: Measurement of Anode Arc Attachment Movement in DC Arc Plasma Torch at Atmospheric Pressure
Author(s): Ondac, P (Ondac, P.); Maslani, A (Maslani, A.); Hrabovsky, M (Hrabovsky, M.); Jenista, J (Jenista, J.)
Source: PLASMA CHEMISTRY AND PLASMA PROCESSING **Volume:** 38 **Issue:** 3 **Pages:** 637-654 **DOI:** 10.1007/s11090-018-9888-0 **Published:** MAY 2018

Abstract: Direct current (DC) arc plasma torches are widely used in various industrial applications. Studying processes in their anode area helps to extend their lifetime, and stabilize the plasma flow for plasma applications. This paper reports detailed observations of the fast movement (above 100 m/s) of the anode arc attachment in a hybrid water-argon DC arc plasma torch with an external anode. We measured a mean electrical conductivity of a plasma volume above the anode and found a relation between the attachment movement and the anode erosion. Further, we measured average attachment speed, the average period of the restrike process and the average distances travelled by the attachment under different experimental conditions such as different values of the arc electric current, argon flow rate and different anode configurations. For our measurements, we used a high-speed camera and a high-voltage probe. Our results are in agreement with a model of plasma generated by a hybrid plasma torch and with spectroscopy measurements. The results describe the movement of the anode arc attachment in detail and provide experimental data on average plasma electrical conductivity in hot anode areas. Both the measurements of the mean electrical conductivity and the procedure for quantitative comparisons of anode erosion can be used also in water plasma torches and theoretically also in gas plasma torches.

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ISSN: 0272-4324
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Record 130 of 214

Title: Microenvironment-driven resistance to B-Raf inhibition in a melanoma patient is accompanied by broad changes of gene methylation and expression in distal fibroblasts

Author(s): Kodet, O (Kodet, Ondrej); Dvorankova, B (Dvorankova, Barbora); Bendlova, B (Bendlova, Bela); Sykorova, V (Sykorova, Vlasta); Krajsova, I (Krajsova, Ivana); Stork, J (Stork, Jiri); Kucera, J (Kucera, Jan); Szabo, P (Szabo, Pavol); Strnad, H (Strnad, Hynek); Kolar, M (Kolar, Michal); Vlcek, C (Vlcek, Cestmir); Smetana, K (Smetana, Karel, Jr.); Lacina, L (Lacina, Lukas)

Source: INTERNATIONAL JOURNAL OF MOLECULAR MEDICINE **Volume:** 41 **Issue:** 5 **Pages:** 2687-2703 **DOI:** 10.3892/ijmm.2018.3448 **Published:** MAY 2018

Abstract: The incidence of malignant melanoma is rapidly increasing and current medicine is offering only limited options for treatment of the advanced disease. For B-Raf mutated melanomas, treatment with mutation-specific drug inhibitors may be used. Unfortunately, tumors frequently acquire resistance to the treatment. Tumor microenvironment, namely cancer-associated fibroblasts, largely influence this acquired resistance. In the present study, fibroblasts were isolated from a patient suffering from acrolentiginous melanoma (Breslow, 4.0 mm; Clark, IV; B-Raf V600E mutated). The present study focused on the expression of structural and functional markers of fibroblast activation in melanoma-associated fibroblasts (MAFs; isolated prior to therapy initiation) as well as in autologous control fibroblasts (ACFs) of the same patient isolated during B-Raf inhibitor therapy, yet before clinical progression of the disease. Analysis of gene transcription was also performed, as well as DNA methylation status analysis at the genomic scale of both isolates. MAFs were positive for smooth muscle actin (SMA), which is a marker of myofibroblasts and the hallmark of cancer stoma. Surprisingly, ACF isolated from the distant uninvolved skin of the same patient also exhibited strong SMA expression. A similar phenotype was also observed in control dermal fibroblasts (CDFs; from different donors) exclusively following stimulation by transforming growth factor (TGF)-1. Immunohistochemistry confirmed that melanoma cells potently produce TGF-1. Significant differences were also identified in gene transcription and in DNA methylation status at the genomic scale. Upregulation of SMA was observed in ACF cells at the protein and transcriptional levels. The present results support recent experimental findings that tumor microenvironment is driving resistance to B-Raf inhibition in patients with melanoma. Such an activated microenvironment may be viable for the growth of circulating melanoma cells.

Accession Number: WOS:000429095900025
PubMed ID: 29393387
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Record 131 of 214

Title: Accurate Binding of Sodium and Calcium to a POPC Bilayer by Effective Inclusion of Electronic Polarization

Author(s): Melcr, J (Melcr, Josef); Martinez-Seara, H (Martinez-Seara, Hector); Nencini, R (Nencini, Ricky); Kolafa, J (Kolafa, Jiri); Jungwirth, P (Jungwirth, Pavel); Ollila, OHS (Ollila, O. H. Samuli)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 122 **Issue:** 16 **Pages:** 4546-4557 **DOI:** 10.1021/acs.jpcb.7b12510 **Published:** APR 26 2018

Abstract: Binding affinities and stoichiometries of Na+ and Ca2+ ions to phospholipid bilayers are of paramount significance in the properties and functionality of cellular membranes. Current estimates of binding affinities and stoichiometries of cations are, however, inconsistent due to limitations in the available experimental and computational methods. In this work, we improve the description of the binding details of Na+ and Ca2+ ions to a 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) bilayer by implicitly including electronic polarization as a mean field correction, known as the electronic continuum correction (ECC). This is applied by scaling the partial charges of a selected state-of-the-art POPC lipid model for molecular dynamics simulations. Our improved ECC-POPC model reproduces not only the experimentally measured structural parameters for the ion-free membrane, but also the response of lipid headgroup to a strongly bound cationic amphiphile, as well as the binding affinities of Na+ and Ca2+ ions. With our new model, we observe on the one side negligible binding of Na+ ions to POPC bilayer, while on the other side stronger interactions of Ca2+ primarily with phosphate oxygens, which is in agreement with the previous interpretations of the experimental spectroscopic data. The present model results in Ca2+ ions forming complexes with one to three POPC molecules with almost equal probabilities, suggesting more complex binding stoichiometries than those from simple models used to interpret the NMR data previously. The results of this work pave the way to quantitative molecular simulations with realistic electrostatic interactions of complex biochemical systems at cellular membranes.

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PubMed ID: 29608850
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Melcr, Josef		0000-0003-4729-3990

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Record 132 of 214

Title: The concept of hybrid molecules of tacrine and benzyl quinolone carboxylic acid (BQCA) as multifunctional agents for Alzheimer's disease

Author(s): Hepnarova, V (Hepnarova, V.); Korabecny, J (Korabecny, J.); Matouskova, L (Matouskova, L.); Jost, P (Jost, P.); Muckova, L (Muckova, L.); Hrabinova, M (Hrabinova, M.); Vykoukalova, N (Vykoukalova, N.); Kerhartova, M (Kerhartova, M.); Kucera, T (Kucera, T.); Dolezal, R (Dolezal, R.); Nepovimova, E (Nepovimova, E.); Spilovska, K (Spilovska, K.); Mezeiova, E (Mezeiova, E.); Pham, NL (Pham, N. L.); Jun, D (Jun, D.); Staud, F (Staud, F.); Kaping, D (Kaping, D.); Kuca, K (Kuca, K.); Soukup, O (Soukup, O.)

Source: EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY **Volume:** 150 **Pages:** 292-306 **DOI:** 10.1016/j.ejmech.2018.02.083 **Published:** APR 25 2018

Abstract: Novel tacrine-benzyl quinolone carboxylic acid (tacrine-BQCA) hybrids were designed based on multi-target directed ligands (MTLDs) paradigm, synthesized and evaluated in vitro as inhibitors of human acetylcholinesterase (hAChE) and human butyrylcholinesterase (hBChE). Tacrine moiety is represented herein as 7-methoxytacrine, 6-chlorotacrine or unsubstituted tacrine forming three different families of seven members, i.e. 21 compounds in overall. Introducing BQCA, a positive modulator of M1 muscarinic acetylcholine receptors (mAChRs), the action of novel compounds on M1 mAChRs was evaluated via Fluo-4 NW assay on the Chinese hamster ovarian (CHO-M1WT2) cell line. All the novel tacrine-BQCA hybrids were able to block the action of hAChE and hBChE in micromolar to nanomolar range. The hAChE kinetic profile of 5p was found to be mixed-type which is consistent with our docking experiments. Moreover, selected ligands were assessed for their potential hepatotoxicity on HepG2 cell line and presumable permeation through the blood-brain barrier by PAMPA assay. Expected agonistic profile towards M1 mAChRs delivered by BQCA moiety was not confirmed. From all the hybrids, 5o can be highlighted as non-selective cholinesterase inhibitor (hAChE IC50 = 74.5 nM; hBChE IC50 = 83.3 nM) with micromolar antagonistic activity towards M1 mAChR (IC50 = 4.23 mu M). A non-selective pattern of cholinesterase inhibition is likely to be valuable during the onset as well as later stages of AD. (C) 2018 Elsevier Masson SAS. All rights reserved.

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Record 133 of 214

Title: Water-Tryptophan Interactions: Lone-pair...pi or O-H...pi? Molecular Dynamics Simulations of beta-Galactosidase Suggest that Both Modes Can Co-exist

Author(s): Durec, M (Durec, Matus); Marek, R (Marek, Radek); Kozelka, J (Kozelka, Jiri)

Abstract: In proteins, the indole side chain of tryptophan can interact with water molecules either in-plane, forming hydrogen bonds, or out-of-plane, with the water molecule contacting the aromatic pi face. The latter interaction can be either of the lone pair...pi (lp...pi) type or corresponds to the O-H...pi binding mode, an ambiguity that X-ray structures usually do not resolve. Here, we report molecular dynamics (MD) simulations of a solvated beta-galactosidase monomer, which illustrate how a water molecule located at the p face of an indole side chain of tryptophan can adapt to the position of proximate residues and "select" its binding mode. In one such site, the water molecule is predicted to rapidly oscillate between the O-H...pi and lp...pi binding modes, thus gaining entropic advantage. Our MD simulations provide support for the role of lp...pi interactions in the stabilization of protein structures.

Accession Number: WOS:000430168500021
PubMed ID: 29315935
Author Identifiers:

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Marek, Radek	D-6929-2012	0000-0002-3668-3523

ISSN: 0947-6539
eISSN: 1521-3765

Record 134 of 214

Title: Stability and elasticity of metastable solid solutions and superlattices in the MoN-TaN system: First-principles calculations

Author(s): Koutna, N (Koutna, Nikola); Holec, D (Holec, David); Friak, M (Friak, Martin); Mayrhofer, PH (Mayrhofer, Paul H.); Sob, M (Sob, Mojmir)

Abstract: In order to develop design rules for novel nitride-based coatings, we investigate trends in thermodynamic, structural, elastic, and electronic properties of $Mo_{1-x}Ta_xN$ single-phase alloys together with $(MoN)_{(1-x)}/(TaN)_{(x)}$ superlattices. Our calculations predict that hexagonal $Mo_{1-x}Ta_xN$ are the overall most stable ones, followed by the disordered cubic solid solutions and superlattices. The disordered cubic systems are energetically clearly favoured over their ordered counterparts. To explain this unexpected phenomenon, we perform an in-depth structural analysis of bond-lengths and angles, revealing that the disordered phase is structurally between the NaCl-type and the hexagonal NiAs-type modifications. Similarly, the bi-axial coherency stresses in MoN/TaN break the cubic symmetry beyond simple tetragonal distortions, leading to a new tetragonal zeta-phase (P4/nmm, #129). Both zeta-MoN and zeta-TaN have lower formation energy than their cubic counterparts. Unlike the cubic TaN, the zeta-TaN is also dynamically stable. The hexagonal alloys are predicted to be extremely hard, though, much less ductile than the cubic polymorphs and superlattices. (C) 2018 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000427609400029
Author Identifiers:

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Sob, Mojmir	D-1936-2012	
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ISSN: 0264-1275
eISSN: 1873-4197

Record 135 of 214

Title: The Lewis acidity of three- and two-dimensional zeolites: The effect of framework topology

Author(s): Ho, TV (Thang Viet Ho); Nachtigall, P (Nachtigall, Petr); Grajciar, L (Grajciar, Lukas)

Abstract: The zeolite activity in processes driven by Lewis acid sites is determined by the distribution of the extra-framework cations in the zeolite and their coordination with the framework (the stronger is the cation coordination, the weaker is its Lewis acidity). This study aims to test how much the transformation from 3D zeolite to its corresponding 2D layered form changes the extra-framework cation distribution and coordination and thus how much it affects the zeolite Lewis acid strength. Zeolites with two distinct topologies, MWW and MFI, which form layers with considerably different silanol density (1.1 and 2.9 silanols/nm(2), respectively) were considered. To probe the Lewis acidity of extra-framework Li+ sites the carbon monoxide stretching frequencies and adsorption enthalpies were calculated, employing the dispersion-corrected density functional theory and the results are in good agreement with available experimental data. No or negligible differences in the Lewis acidity of Li+ sites in 2D and 3D form of zeolites with MWW topology are found; both, the extra-framework cation distribution and the coordination with the framework remain the same. On the contrary, there are significant differences in Lewis acidic properties of 3D and 2D zeolites with MFI topology. The Li+ cation coordination in 2D-MFI is considerably improved compared to 3D-MFI due to the large concentration of surface silanols and due to an increased flexibility of the material. Consequently, Lewis acidity of 2D-MFI is lower compared to corresponding 3D-MFI material. This Lewis acidity decrease also reflects the fact that the strongest Lewis acid sites found in 3D zeolite - the channel-intersection sites (coordinated with two framework oxygens only) - are not present in 2D-MFI. The results reported herein suggest that the flexibility of the layer, which increases with silanol density and varies for each zeolite topology, significantly influences its Lewis acidity; the larger is the flexibility of the layer, the better is the cation coordination with the framework and thus smaller is its Lewis acidity.

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Conference Title: 7th Czech-Italian-Spanish Symposium on Zeolites and Catalysis
Conference Date: JUN, 2017
Conference Location: CZECH REPUBLIC
Author Identifiers:

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Grajciar, Lukas		0000-0001-9464-7769

ISSN: 0920-5861
eISSN: 1873-4308

Record 136 of 214

Title: Global hot-star wind models for stars from Magellanic Clouds

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

Abstract: We provide mass-loss rate predictions for O stars from Large and Small Magellanic Clouds. We calculate global (unified, hydrodynamic) model atmospheres of main sequence, giant, and supergiant stars for chemical composition corresponding to Magellanic Clouds. The models solve radiative transfer equation in comoving frame, kinetic equilibrium equations (also known as NLTE equations), and hydrodynamical equations from (quasi-)hydrostatic atmosphere to expanding stellar wind. The models allow us to predict wind density, velocity, and temperature (consequently also the terminal wind velocity and the mass-loss rate) just from basic global stellar parameters. As a result of their lower metallicity, the line radiative driving is weaker leading to lower wind mass-loss rates with respect to the Galactic stars. We provide a formula that fits the mass-loss rate predicted by our models as a function of stellar luminosity and metallicity. On average, the mass-loss rate scales with metallicity as. (M) over dot similar to Z(0.59). The predicted mass-loss rates are lower than mass-loss rates derived from Hff diagnostics and can be reconciled with observational results assuming clumping factor C-c = 9. On the other hand, the predicted mass-loss rates either agree or are slightly higher than the mass-loss rates derived from ultraviolet wind line profiles. The calculated P V ionization fractions also agree with values derived from observations for LMC stars with T-eff <= 40 000 K. Taken together, our theoretical predictions provide reasonable models with consistent mass-loss rate determination, which can be used for quantitative study of stars from Magellanic Clouds.

Accession Number: WOS:000430139600001
Author Identifiers:

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

ISSN: 1432-0746

Record 137 of 214

Title: Identification of Eukaryotic Translation Elongation Factor 1-alpha 1 Gamendazole-Binding Site for Binding of 3-Hydroxy-4(1&ITH&IT)-quinolinones as Novel Ligands with Anticancer Activity

Author(s): Burglova, K (Burglova, Kristyna); Rylova, G (Rylova, Gabriela); Markos, A (Markos, Athanasios); Prichystalova, H (Prichystalova, Hana); Soural, M (Soural, Miroslav); Petracek, M (Petracek, Marek); Medvedikova, M (Medvedikova, Martina); Tejral, G (Tejral, Gracian); Sopko, B (Sopko, Bruno); Hradil, P (Hradil, Pavel); Dzubak, P (Dzubak, Petr); Hajduch, M (Hajduch, Marian); Hlavac, J (Hlavac, Jan)

Source: JOURNAL OF MEDICINAL CHEMISTRY **Volume:** 61 **Issue:** 7 **Pages:** 3027-3036 **DOI:** 10.1021/acs.jmedchem.8b00078 **Published:** APR 12 2018

Abstract: Here, we have identified the interaction site of the contraceptive drug gamendazole using computational modeling. The drug was previously described as a ligand for eukaryotic translation elongation factor 1-alpha 1 (eEF1A1) and found to be a potential target site for derivatives of 2-phenyl-3-hydroxy-4(1H)-quinolinones (3-HQs), which exhibit anticancer activity. The interaction of this class of derivatives of 3-HQs with eEF1A1 inside cancer cells was confirmed via pull-down assay. We designed and synthesized a new family of 3-HQs and subsequently applied isothermal titration calorimetry to show that these compounds strongly bind to eEF1A1. Further, we found that some of these derivatives possess significant in vitro anticancer activity.

Accession Number: WOS:000430256600026
PubMed ID: 29498519
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ISSN: 0022-2623
eISSN: 1520-4804

Record 138 of 214
Title: Interactions of Ascorbic Acid with Satraplatin and its trans Analog JM576: DFT Computational Study
Author(s): Sebesta, F (Sebesta, Filip); Burda, JV (Burda, Jaroslav V.)
Source: EUROPEAN JOURNAL OF INORGANIC CHEMISTRY **Issue:** 13 **Pages:** 1481-1491 **DOI:** 10.1002/ejic.201701334 **Published:** APR 9 2018

Abstract: Knowledge of the mechanisms for the reduction of Pt-IV anticancer prodrugs is of great importance, since the reduction process is considered as a necessary step for their activation. Therefore, in this study, we investigate the reduction of satraplatin {JM216, cis,trans,cis-[PtCl2(OAc)(2)(cha)(NH3)], cha = cyclohexylamine} by ascorbic acid (AA) where proton-assisted electron-transfer and outer-sphere electron-transfer mechanisms are employed. Also, the presence of an additional base, which should increase the concentration of the deprotonated AA(2-) form, is discussed. Structures are optimized at the B3LYP-GD3BJ/6-31+G(d)/MWB60/C-PCM/Klamt level and single-point calculations are performed in the larger 6-311++G(2df,2pd)/MWB60 basis set, together with the better implicit solvation model - IEF-PCM/scaled-UAKS. All three protonation states of ascorbic acid are taken into consideration. An effective rate constant of 2.6x10(-3) m(-1)s(-1) is obtained from the kinetic formalism for side reactions, as described recently. For the reduction of satraplatin by fully deprotonated ascorbic acid, changes of the electron-density distribution along the reaction coordinate are further investigated using NPA, QTAIM, and reaction electronic-flux analysis. Both electron-transfer mechanisms are also explored for the satraplatin trans analog JM576 {trans,trans,trans-[PtCl2(OAc)(2)(cha)(NH3)]}. The resulting effective rate constant of 5.1x10(-2) m(-1)s(-1) is compared with available experimental data.

Accession Number: WOS:000430003700003
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bUrda, Jaroslav		0000-0001-9909-8797

ISSN: 1434-1948
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Record 139 of 214
Title: Excitonic magnet in external field: Complex order parameter and spin currents
Author(s): Geffroy, D (Geffroy, D.); Hariki, A (Hariki, A.); Kunes, J (Kunes, J.)
Source: PHYSICAL REVIEW B **Volume:** 97 **Issue:** 15 **Article Number:** 155114 **DOI:** 10.1103/PhysRevB.97.155114 **Published:** APR 9 2018

Abstract: We investigate spin-triplet exciton condensation in the two-orbital Hubbard model close to half-filling by means of dynamical mean-field theory. Employing an impurity solver that handles complex off-diagonal hybridization functions, we study the behavior of excitonic condensate in stoichiometric and doped systems subject to external magnetic field. We find a general tendency of the triplet order parameter to lie perpendicular with the applied field and identify exceptions from this rule. For solutions exhibiting k-odd spin textures, we discuss the Bloch theorem, which, in the absence of spin-orbit coupling, forbids the appearance of spontaneous net spin current. We demonstrate that the Bloch theorem is not obeyed by the dynamical mean-field theory.

Accession Number: WOS:000429455400001
Author Identifiers:

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Kunes, Jan	B-4484-2008	0000-0001-9682-7640

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eISSN: 2469-9969

Record 140 of 214
Title: Novel photocatalytic water splitting solar-to-hydrogen energy conversion: CdLa2S4 and CdLa2Se4 ternary semiconductor compounds
Author(s): Reshak, AH (Reshak, A. H.)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 20 **Issue:** 13 **Pages:** 8848-8858 **DOI:** 10.1039/c8cp00373d **Published:** APR 7 2018

Abstract: Comprehensive ab initio calculations from first- to second-principles methods are performed to investigate the suitability of non-centro-symmetric CdLa2S4 and CdLa2Se4 to be used as active photocatalysts under visible light illumination. The calculations reveal the direct band gap nature of both compounds with large absorption coefficients (10(4)-10(5) cm(-1)). The absorption edges of CdLa2S4 and CdLa2Se4 occur at = 579.3 nm and = 670.1 nm, and the optical band gaps are estimated to be 2.14 eV and 1.85 eV for CdLa2S4 and CdLa2Se4, respectively. These gaps are larger than 1.23 eV the required optical band gap for photocatalytic performance to split water under visible light illumination. The calculated potentials of the conduction band and the valence band edges indicate that CdLa2S4 and CdLa2Se4 have strong reducing powers for H-2 production. The obtained results reveal that the high photogenerated carrier mobility favors enhancement of the photocatalytic performance. It has been found that there is a large mobility difference between the electrons (e(-)) and the holes (h(+)), which is useful for the separation of e(-) and h(+), reduction of e(-) and h(+) recombination rate, and improvement of the photocatalytic activity. Based on these findings, one can conclude that CdLa2S4 and CdLa2Se4 satisfied all requirements to be efficient photocatalysts. This will greatly improve the search efficiency and greatly help experiments to save resources in the exploration of new photocatalysts with good photocatalytic performances.

Accession Number: WOS:000428779700047
PubMed ID: 29542783
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Author	ResearcherID Number	ORCID Number
Reshak, A		0000-0001-9426-8363

ISSN: 1463-9076
eISSN: 1463-9084

Record 141 of 214
Title: Calcium Sensing by Recoverin: Effect of Protein Conformation on Ion Affinity
Author(s): Timr, S (Timr, Stepan); Kadlec, J (Kadlec, Jan); Srb, P (Srb, Pavel); Ollila, OHS (Ollila, O. H. Samuli); Jungwirth, P (Jungwirth, Pavel)
Source: JOURNAL OF PHYSICAL CHEMISTRY LETTERS **Volume:** 9 **Issue:** 7 **Pages:** 1613-1619 **DOI:** 10.1021/acs.jpclett.8b00495 **Published:** APR 5 2018

Abstract: The detailed functional mechanism of recoverin, which acts as a myristoyl switch at the rod outer-segment disk membrane, is elucidated by direct and replica-exchange molecular dynamics. In accord with NMR structural evidence and calcium binding assays, simulations point to the key role of enhanced calcium binding to the EF3 loop of the semiopen state of recoverin as compared to the closed state. This 2-4-order decrease in calcium dissociation constant stabilizes the semiopen state in response to the increase of cytosolic calcium concentration in the vicinity of recoverin. A second calcium ion then binds to the EF2 loop and, consequently, the structure of the protein changes from the semiopen

to the open state. The latter has the myristoyl chain extruded to the cytosol, ready to act as a membrane anchor of recoverin.

Accession Number: WOS:000429626900023

PubMed ID: 29537287

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Timr, Stepan		0000-0002-5824-4476

ISSN: 1948-7185

Record 142 of 214

Title: CD9 and CD81 Interactions and Their Structural Modelling in Sperm Prior to Fertilization

Author(s): Frolikova, M (Frolikova, Michaela); Manaskova-Postlerova, P (Manaskova-Postlerova, Pavla); Cerny, J (Cerny, Jiri); Jankovicova, J (Jankovicova, Jana); Simonik, O (Simonik, Ondrej); Pohlova, A (Pohlova, Alzbeta); Secova, P (Secova, Petra); Antalikova, J (Antalikova, Jana); Dvorakova-Hortova, K (Dvorakova-Hortova, Katerina)

Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES **Volume:** 19 **Issue:** 4 **Article Number:** 1236 **DOI:** 10.3390/ijms19041236 **Published:** APR 2018

Abstract: Proteins CD9 and CD81 are members of the tetraspanin superfamily and were detected in mammalian sperm, where they are suspected to form an active tetraspanin web and to participate in sperm-egg membrane fusion. The importance of these two proteins during the early stages of fertilization is supported by the complete sterility of CD9/CD81 double null female mice. In this study, the putative mechanism of CD9/CD81 involvement in tetraspanin web formation in sperm and its activity prior to fertilization was addressed. Confocal microscopy and colocalization assay was used to determine a mutual CD9/CD81 localization visualised in detail by super-resolution microscopy, and their interaction was address by co-immunoprecipitation. The species-specific traits in CD9 and CD81 distribution during sperm maturation were compared between mice and humans. A mutual position of CD9/CD81 is shown in human spermatozoa in the acrosomal cap, however in mice, CD9 and CD81 occupy a distinct area. During the acrosome reaction in human sperm, only CD9 is relocated, compared to the relocation of both proteins in mice. The structural modelling of CD9 and CD81 homologous and possibly heterologous network formation was used to propose their lateral Cis as well as Trans interactions within the sperm membrane and during sperm-egg membrane fusion.

Accession Number: WOS:000434978700315

PubMed ID: 29671763

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Antalikova, Jana		0000-0002-6617-6485
Jankovicova, Jana		0000-0002-4714-6184

ISSN: 1422-0067

Record 143 of 214

Title: The Didymodon tophaceus complex (Pottiaceae, Bryophyta) revisited: new data support the subspecific rank of currently recognized species

Author(s): Kucera, J (Kucera, Jan); Blockeel, TL (Blockeel, Tom L.); Erzberger, P (Erzberger, Peter); Papp, B (Papp, Beata); Soldan, Z (Soldan, Zdenek); Vellak, K (Vellak, Kai); Werner, O (Werner, Olaf); Ros, RM (Ros, Rosa M.)

Source: CRYPTOGAMIE BRYOLOGIE **Volume:** 39 **Issue:** 2 **Pages:** 241-257 **DOI:** 10.7872/cryb/v39.iss2.2018.241 **Published:** APR 2018

Abstract: Additional samples of Didymodon erosus and D. sicculus, barcoded using ITS sequences, necessitated the broadening of the morphological concepts and the reported ecology of these taxa, both of which were revealed to have considerable overlap. Additional molecular data from the chloroplast genome confirmed the earlier published phylogenetic inference based on the nuclear ITS, which groups Didymodon tophaceus, Didymodon erosus and D. sicculus into a highly supported lineage of closely related taxa. In view of the morphological overlap among taxa of the D. tophaceus complex, supported by the ITS non-monophyly of D. tophaceus in its current morphological concept, we advocate the reduction of D. erosus and D. sicculus to infraspecific rank within D. tophaceus. Sporophytes are described for the first time in D. erosus, and new country records for the latter two taxa are reported.

Accession Number: WOS:000430832200014

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Kucera, Jan	B-3633-2009	0000-0002-0230-5997

ISSN: 1290-0796

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Record 144 of 214

Title: Exploration of selected electronic characteristics of half-sandwich organoruthenium(II) beta-diketonate complexes

Author(s): Vokacova, ZS (Vokacova, Zuzana Sochorova); Turel, I (Turel, Iztok); Burda, JV (Burda, Jaroslav V.)

Source: JOURNAL OF MOLECULAR MODELING **Volume:** 24 **Issue:** 4 **Article Number:** 98 **DOI:** 10.1007/s00894-018-3598-7 **Published:** APR 2018

Abstract: Based on experimental work, 12 half-sandwich organoruthenium(II) complexes with p-cymene and various substituted beta-diketonates (acac) modified by several functional groups were explored. These complexes were optimized at the B3PW91/6-31 + G(d)/PCM/UFF computational level with the Ru atom described by Stuttgart pseudopotentials. The electron density analysis was performed using the B3LYP/6-311++G(2df, 2pd)/DPCM/scaled-UAKS model. Electrostatic and averaged local ionization potential were explored and extremes on 0.001 e/a.u.(3) isodensity surfaces discussed. Natural population analysis partial charges and electron densities in bond critical point of the key Ru(II) coordination bonds were determined. There was a clear correlation between the results obtained and experimentally known anticancer descriptors.

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PubMed ID: 29556743

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Sochorova Vokacova, Zuzana	O-4878-2018	
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ISSN: 1610-2940

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Record 145 of 214

Title: Asteroid clusters similar to asteroid pairs

Author(s): Pravec, P (Pravec, P.); Fatka, P (Fatka, P.); Vokrouhlicky, D (Vokrouhlicky, D.); Scheeres, DJ (Scheeres, D. J.); Kusnirak, P (Kusnirak, P.); Hornoch, K (Hornoch, K.); Galad, A (Galad, A.); Vrastil, J (Vrastil, J.); Pray, DP (Pray, D. P.); Krugly, YN (Krugly, Yu. N.); Gaftonyuk, NM (Gaftonyuk, N. M.); Inasaridze, RY (Inasaridze, R. Ya.); Ayvazian, VR (Ayvazian, V. R.); Kvaratskhelia, OI (Kvaratskhelia, O. I.); Zhuzhunadze, VT (Zhuzhunadze, V. T.); Husarik, M (Husarik, M.); Cooney, WR (Cooney, W. R.); Gross, J (Gross, J.); Terrell, D (Terrell, D.); Vilagi, J (Vilagi, J.); Kornos, L (Kornos, L.); Gajdos, S (Gajdos, S.); Burkhonov, O (Burkhonov, O.); Ehgamberdiev, SA (Ehgamberdiev, Sh. A.); Donchev, Z (Donchev, Z.); Borisov, G (Borisov, G.); Bonev, T (Bonev, T.); Rumyantsev, VV (Rumyantsev, V. V.); Molotov, IE (Molotov, I. E.)

Source: ICARUS **Volume:** 304 **Pages:** 110-126 **DOI:** 10.1016/j.icarus.2017.08.008 **Published:** APR 2018

Abstract: We studied the membership, size ratio and rotational properties of 13 asteroid clusters consisting of between 3 and 19 known members that are on similar heliocentric orbits. By backward integrations of their orbits, we confirmed their cluster membership and estimated times elapsed since separation of the secondaries (the smaller cluster members) from the primary (i.e., cluster age) that are between 105 and a few 106 years. We ran photometric observations for all the cluster primaries and a sample of secondaries and we derived their accurate absolute magnitudes and rotation periods. We found that 11 of the 13 clusters follow the same trend of primary rotation period vs mass ratio as asteroid pairs that was revealed by Pravec et al. (2010). We generalized the model of the post-fission system for asteroid pairs by Pravec et al. (2010) to a system of N components formed by rotational fission and we found excellent agreement between the data for the 11 asteroid clusters and the prediction from the theory of their formation by rotational fission. The two exceptions are the

high-mass ratio (q > 0.7) clusters of (18777) Hobson and (22280) Mandragora for which a different formation mechanism is needed. Two candidate mechanisms for formation of more than one secondary by rotational fission were published: the secondary fission process proposed by Jacobson and Scheeres (2011) and a cratering collision event onto a nearly critically rotating primary proposed by Vokrouhlick et al. (2017). It will have to be revealed from future studies which of the clusters were formed by one or the other process. To that point, we found certain further interesting properties and features of the asteroid clusters that place constraints on the theories of their formation, among them the most intriguing being the possibility of a cascade disruption for some of the clusters. (C) 2017 Elsevier Inc. All rights reserved.

Accession Number: WOS:000426535800012

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Record 146 of 214
Title: Computer-assisted engineering of hyperstable fibroblast growth factor 2
Author(s): Dvorak, P (Dvorak, Pavel); Bednar, D (Bednar, David); Vanacek, P (Vanacek, Pavel); Balek, L (Balek, Lukas); Eiselleova, L (Eiselleova, Livia); Stepankova, V (Stepankova, Veronika); Sebestova, E (Sebestova, Eva); Bosakova, MK (Bosakova, Michaela Kunova); Konecna, Z (Konecna, Zaneta); Mazurenko, S (Mazurenko, Stanislav); Kunka, A (Kunka, Antonin); Vanova, T (Vanova, Tereza); Zoufalova, K (Zoufalova, Karolina); Chaloupkova, R (Chaloupkova, Radka); Brezovsky, J (Brezovsky, Jan); Krejci, P (Krejci, Pavel); Prokop, Z (Prokop, Zbynek); Dvorak, P (Dvorak, Petr); Damborsky, J (Damborsky, Jiri)
Source: BIOTECHNOLOGY AND BIOENGINEERING **Volume:** 115 **Issue:** 4 **Pages:** 850-862 **DOI:** 10.1002/bit.26531 **Published:** APR 2018

Abstract: Fibroblast growth factors (FGFs) serve numerous regulatory functions in complex organisms, and their corresponding therapeutic potential is of growing interest to academics and industrial researchers alike. However, applications of these proteins are limited due to their low stability. Here we tackle this problem using a generalizable computer-assisted protein engineering strategy to create a unique modified FGF2 with nine mutations displaying unprecedented stability and uncompromised biological function. The data from the characterization of stabilized FGF2 showed a remarkable prediction potential of in silico methods and provided insight into the unfolding mechanism of the protein. The molecule holds a considerable promise for stem cell research and medical or pharmaceutical applications.

Accession Number: WOS:000426493300005
PubMed ID: 29278409

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Damborsky, Jiri	H-3799-2012	0000-0002-7848-8216
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ISSN: 0006-3592
eISSN: 1097-0290

Record 147 of 214
Title: Dominance of hole-boring radiation pressure acceleration regime with thin ribbon of ionized solid hydrogen
Author(s): Psikal, J (Psikal, J.); Matys, M (Matys, M.)
Source: PLASMA PHYSICS AND CONTROLLED FUSION **Volume:** 60 **Issue:** 4 **Article Number:** 044003 **DOI:** 10.1088/1361-6587/aaa7fa **Published:** APR 2018

Abstract: Laser-driven proton acceleration from novel cryogenic hydrogen target of the thickness of tens of microns irradiated by multiPW laser pulse is investigated here for relevant laser parameters accessible in near future. It is demonstrated that the efficiency of proton acceleration from relatively thick hydrogen solid ribbon largely exceeds the acceleration efficiency for a thinner ionized plastic foil, which can be explained by enhanced hole boring (HB) driven by laser ponderomotive force in the case of light ions and lower target density. Three-dimensional particle-in-cell (PIC) simulations of laser pulse interaction with relatively thick hydrogen target show larger energies of protons accelerated in the target interior during the HB phase and reduced energies of protons accelerated from the rear side of the target by quasistatic electric field compared with the results obtained from two-dimensional PIC calculations. Linearly and circularly polarized multiPW laser pulses of duration exceeding 100 fs show similar performance in terms of proton acceleration from both the target interior as well as from the rear side of the target. When ultrashort pulse (similar to 30 fs) is assumed, the number of accelerated protons from the target interior is substantially reduced.

Accession Number: WOS:000424775600002

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Psikal, Jan		0000-0003-4586-1149

ISSN: 0741-3335
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Record 148 of 214
Title: The Sub-Regional Functional Organization of Neocortical Irritative Epileptic Networks in Pediatric Epilepsy
Author(s): Janca, R (Janca, Radek); Krsek, P (Krsek, Pavel); Jezdik, P (Jezdik, Petr); Cmejla, R (Cmejla, Roman); Tomasek, M (Tomasek, Martin); Komarek, V (Komarek, Vladimir); Marusic, P (Marusic, Petr); Jiruska, P (Jiruska, Premysl)
Source: FRONTIERS IN NEUROLOGY **Volume:** 9 **Article Number:** 184 **DOI:** 10.3389/fneur.2018.00184 **Published:** MAR 23 2018

Abstract: Between seizures, irritative network generates frequent brief synchronous activity, which manifests on the EEG as interictal epileptiform discharges (IEDs). Recent insights into the mechanism of IEDs at the microscopic level have demonstrated a high variance in the recruitment of neuronal populations generating IEDs and a high variability in the trajectories through which IEDs propagate across the brain. These phenomena represent one of the major constraints for precise characterization of network organization and for the utilization of IEDs during presurgical evaluations. We have developed a new approach to dissect human neocortical irritative networks and quantify their properties. We have demonstrated that irritative network has modular nature and it is composed of multiple the extent of IED activity generated. The global activity of the irritative network is determined by long-term and circadian fluctuations in sub-region spatiotemporal properties. Also, the most active sub-region co-localizes with the seizure onset zone in 12/14 cases. This study demonstrates that principles of recruitment variability and propagation are conserved at the macroscopic level and that they determine irritative network properties in humans. Functional stratification of the irritative network increases the diagnostic yield of intracranial investigations with the potential to improve the outcomes of surgical treatment of neocortical epilepsy.

Accession Number: WOS:000428191100001
PubMed ID: 29628910

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Jiruska, Premysl		0000-0003-4955-8577
Janca, Radek		0000-0003-0825-1069

Record 149 of 214

Title: Nonconjugated Acyloxy Group Deactivates the Intramolecular Charge-Transfer State in the Carotenoid Fucoxanthin

Author(s): Staleva-Musto, H (Staleva-Musto, Hristina); Kuznetsova, V (Kuznetsova, Valentyna); West, RG (West, Robert G.); Kesan, G (Kesan, Gurkan); Minofar, B (Minofar, Babak); Fuciman, M (Fuciman, Marcel); Bina, D (Bina, David); Litvin, R (Litvin, Radek); Polivka, T (Polivka, Tomas)

Abstract: We used ultrafast transient absorption spectroscopy to study excited-state dynamics of the keto-carotenoid fucoxanthin (Fx) and its two derivatives: 19'-butanoyloxyfucoxanthin (bFx) and 19'-hexanoyloxyfucoxanthin (hFx). These derivatives occur in some light harvesting systems of photosynthetic microorganisms, and their presence is typically related to stress conditions. Even though the hexanoyl (butanoyl) moiety is not a part of the conjugated system of hFx (bFx), their absorption spectra in polar solvents exhibit more pronounced vibrational bands of the S-2 state than for Fx. The effect of the nonconjugated acyloxy moiety is further observed in transient absorption spectra, which for Fx exhibit characteristic features of an intramolecular charge transfer (ICT) state in all polar solvents. For bFx and hFx, however, much weaker ICT features are detected in methanol, and the spectral markers of the ICT state disappear completely in polar, but aprotic acetonitrile. The presence of the acyloxy moiety also alters the lifetimes of the S-1/ICT state. For Fx, the lifetimes are 60, 30, and 20 ps in n-hexane, acetonitrile, and methanol, whereas for bFx and hFx, these lifetimes yield 60, 60, and 40 ps, respectively. Testing the S-1/ICT state lifetimes of hFx in other solvents revealed that some ICT features can be induced only in polar, protic solvents (methanol, ethanol, and ethylene glycol). Thus, bFx and hFx represent a rather rare example of a system in which a nonconjugated functional group significantly alters excited-state dynamics. By comparison with other carotenoids, we show that a keto group at the acyloxy tail, even though it is not in conjugation, affects the electron distribution along the conjugated backbone, resulting in the observed decrease of the ICT character of the S-1/ICT state of bFx and hFx.

Accession Number: WOS:000428356900009

PubMed ID: 29469573

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Litvin, Radek	G-8502-2014	0000-0001-5272-9029
KESAN, Gurkan		0000-0002-7812-6872
Minofar, Babak		0000-0001-8096-2194

Record 150 of 214

Title: Transport theory for femtosecond laser-induced spin-transfer torques

Author(s): Balaz, P (Balaz, Pavel); Zonda, M (Zonda, Martin); Carva, K (Carva, Karel); Maldonado, P (Maldonado, Pablo); Oppeneer, PM (Oppeneer, Peter M.)

Abstract: Ultrafast demagnetization of magnetic layers pumped by a femtosecond laser pulse is accompanied by a nonthermal spin-polarized current of hot electrons. These spin currents are studied here theoretically in a spin valve with noncollinear magnetizations. To this end, we introduce an extended model of superdiffusive spin transport that enables the treatment of noncollinear magnetic configurations, and apply it to the perpendicular spin valve geometry. We show how spin-transfer torques arise due to this mechanism and calculate their action on the magnetization, as well as how the latter depends on the thicknesses of the layers and other transport parameters. We demonstrate that there exists a certain optimum thickness of the out-of-plane magnetized spin-current polarizer such that the torque acting on the second magnetic layer is maximal. Moreover, we study the magnetization dynamics excited by the superdiffusive spin-transfer torque due to the flow of hot electrons employing the Landau-Lifshitz-Gilbert equation. Thereby we show that a femtosecond laser pulse applied to one magnetic layer can excite small-angle precessions of the magnetization in the second magnetic layer. We compare our calculations with recent experimental results.

Accession Number: WOS:000425996100001

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Balaz, Pavel	M-9510-2015	0000-0003-0016-9271
Maldonado, Pablo		0000-0002-8524-819X
Oppeneer, Peter		0000-0002-9069-2631

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Record 151 of 214

Title: How Does a Container Affect Acidity of its Content: Charge-Depletion Bonding Inside Fullerenes

Author(s): Jaros, A (Jaros, Adam); Badri, Z (Badri, Zahra); Bora, PL (Bora, Pankaj Lochan); Bonab, EF (Bonab, Esmaeil Farajpour); Marek, R (Marek, Radek); Straka, M (Straka, Michal); Foroutan-Nejad, C (Foroutan-Nejad, Cina)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 24 **Issue:** 17 **Pages:** 4245-4249 **DOI:** 10.1002/chem.201706017 **Published:** MAR 20 2018

Abstract: A recent study (Sci. Adv. 2017, 3, e1602833) has shown that FHOH2 hydrogen bond in a HFH2O pair substantially shortens, and the H-F bond elongates upon encapsulation of the cluster in C-70 fullerene. This has been attributed to compression of the HFH2O pair inside the cavity of C-70. Herein, we present theoretical evidence that the effect is not caused by a mere compression of the H2OHF pair, but it is related to a strong lone-pair- (LP-) bonding with the fullerene cage. To support this argument, a systematic electronic structure study of selected small molecules (HF, H2O, and NH3) and their pairs enclosed in fullerene cages (C-60, C-70, and C-90) has been performed. Bonding analysis revealed unique LP-(cage) interactions with a charge-depletion character in the bonding region, unlike usual LP- bonds. The LP-(cage) interactions were found to be responsible for elongation of the H-F bond. Thus, the HF appears to be more acidic inside the cage. The shortening of the FHOH2 contact in (HFH2O)@C-70 originates from an increased acidity of the HF inside the fullerenes. Such trends were also observed in other studied systems.

Accession Number: WOS:000428376900008

PubMed ID: 29431245

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Straka, Michal		0000-0002-7857-4990

ISSN: 0947-6539

eISSN: 1521-3765

Record 152 of 214

Title: Aggregation and metal-complexation behaviour of THPP porphyrin in ethanol/water solutions as function of pH

Author(s): Zannotti, M (Zannotti, Marco); Giovannetti, R (Giovannetti, Rita); Minofar, B (Minofar, Babak); Reha, D (Reha, David); Plackova, L (Plackova, Lydie); D'Amato, CA (D'Amato, Chiara A.); Rommozzi, E (Rommozzi, Elena); Dudko, HV (Dudko, Hanna V.); Kari, N (Kari, Nuerguli); Minicucci, M (Minicucci, Marco)

Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 193 **Pages:** 235-248 **DOI:** 10.1016/j.saa.2017.12.021 **Published:** MAR 15 2018

Abstract: The effect of pH change on 5,10,15,20-Tetrakis(4-hydroxypheny1)-21H,23H-porphine (THPP) with its aggregation as function of water-ethanol mixture was studied with UV-vis, fluorescence, Raman and computational analysis. In neutral pH, THPP was present as free-base and, increasing the water amount, aggregation occurred with the formation of H- and J-aggregates. The aggregation constant and the concentration of dimers were calculated, other information about the dimer aggregation were evaluated by computational study. In acidic pH, by the insertions of two hydrogens in the porphyrin rings, the porphyrin changed its geometry with a ring deformation confirmed by red-shifted spectrum and quenching in fluorescence; at this low pH, increasing the water amount, the acidic form (THPPH2)(2+) resulted more stable due to a polar environment with stronger interaction by hydrogen bonding.

In basic pH, reached by NH4OH, THPP porphyrin was able to react with alkali metals in order to form sitting-atop complex (M2THPP) confirmed by the typical absorption spectrum of metallo-porphyrin, Raman spectroscopy and by computational analysis. (C) 2017 Elsevier B.V. All rights reserved.

Accession Number: WOS:000424962900031

PubMed ID: 29247920

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Minofar, Babak		0000-0001-8096-2194
Rommozzi, Elena		0000-0003-2497-0768

ISSN: 1386-1425

Record 153 of 214

Title: Microscopic multiphonon approach to spectroscopy in the neutron-rich oxygen region

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:** 97 **Issue:** 3 **Article Number:** 034311 **DOI:** 10.1103/PhysRevC.97.034311 **Published:** MAR 8 2018

Abstract: Background: A fairly rich amount of experimental spectroscopic data have disclosed intriguing properties of the nuclei in the region of neutron rich oxygen isotopes up to the neutron dripline. They, therefore, represent a unique laboratory for studying the evolution of nuclear structure away from the stability line.

Purpose: We intend to give an exhaustive microscopic description of low and high energy spectra, dipole response, weak, and electromagnetic properties of the even O-22 and the odd O-23 and F-23.

Method: An equation of motion phonon method generates an orthonormal basis of correlated n-phonon states (n = 0,1,2,...) built of constituent Tamm-Dancoff phonons. This basis is adopted to solve the full eigenvalue equations in even nuclei and to construct an orthonormal particle-core basis for the eigenvalue problem in odd nuclei. No approximations are involved and the Pauli principle is taken into full account. The method is adopted to perform self-consistent, parameter free, calculations using an optimized chiral nucleon-nucleon interaction in a space encompassing up to two-phonon basis states.

Results: The computed spectra in O-22 and O-23 and the dipole cross section in O-22 are in overall agreement with the experimental data. The calculation describes poorly the spectrum of F-23.

Conclusions: The two-phonon configurations play a crucial role in the description of spectra and transitions. The large discrepancies concerning the spectra of F-23 are ultimately traced back to the large separation between the Hartree-Fock levels belonging to different major shells. We suggest that a more compact single particle spectrum is needed and can be generated by a new chiral potential which includes explicitly the contribution of the three-body forces.

Accession Number: WOS:000426902800001

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Author	ResearcherID Number	ORCID Number
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ISSN: 2469-9985

eISSN: 2469-9993

Record 154 of 214

Title: Band structure of CuMnAs probed by optical and photoemission spectroscopy

Author(s): Veis, M (Veis, M.); Minar, J (Minar, J.); Steciuk, G (Steciuk, G.); Palatinus, L (Palatinus, L.); Rinaldi, C (Rinaldi, C.); Cantoni, M (Cantoni, M.); Kriegner, D (Kriegner, D.); Tikuisis, KK (Tikuisis, K. K.); Hamrle, J (Hamrle, J.); Zahradnik, M (Zahradnik, M.); Antos, R (Antos, R.); Zelezny, J (Zelezny, J.); Smejkal, L (Smejkal, L.); Marti, X (Marti, X.); Wadley, P (Wadley, P.); Campion, RP (Campion, R. P.); Frontera, C (Frontera, C.); Uhlirova, K (Uhlirova, K.); Duchon, T (Duchon, T.); Kuzel, P (Kuzel, P.); Novak, V (Novak, V.); Jungwirth, T (Jungwirth, T.); Vyborny, K (Vyborny, K.)

Source: PHYSICAL REVIEW B **Volume:** 97 **Issue:** 12 **Article Number:** 125109 **DOI:** 10.1103/PhysRevB.97.125109 **Published:** MAR 8 2018

Abstract: The tetragonal phase of CuMnAs progressively appears as one of the key materials for antiferromagnetic spintronics due to efficient current-induced spin-torques whose existence can be directly inferred from crystal symmetry. Theoretical understanding of spintronic phenomena in this material, however, relies on the detailed knowledge of electronic structure (band structure and corresponding wave functions) which has so far been tested only to a limited extent. We show that AC permittivity (obtained from ellipsometry) and UV photoelectron spectra agree with density functional calculations. Together with the x-ray diffraction and precession electron diffraction tomography, our analysis confirms recent

theoretical claim [Phys. Rev. B 96, 094406 (2017)] that copper atoms occupy lattice positions in the basal plane of the tetragonal unit cell.

Accession Number: WOS:000426902400004

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Minar, Jan	O-3186-2013	0000-0001-9735-8479
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Kriegner, Dominik	C-6225-2013	0000-0001-6961-6581
Kuzel, Petr	G-6006-2014	0000-0003-1134-9198
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Jungwirth, Tomas	G-8952-2014	0000-0002-9910-1674

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Record 155 of 214

Title: Adsorption of amphiphilic graft copolymers in solvents selective for the grafts on a lyophobic surface: a coarse-grained simulation study

Author(s): Posel, Z (Posel, Zbysek); Svoboda, M (Svoboda, Martin); Limpouchova, Z (Limpouchova, Zuzana); Lisal, M (Lisal, Martin); Prochazka, K (Prochazka, Karel)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 20 **Issue:** 9 **Pages:** 6533-6547 **DOI:** 10.1039/c7cp08327k **Published:** MAR 7 2018

Abstract: The sorption of graft copolymers on surfaces attractive only for the backbone and its effect on the conformational behavior of adsorbed/desorbed chains in solvents good for the grafts and poor for the backbone was studied by coarse-grained computer simulations. It was found that the sorption and conformational behavior are very complex and are results of an intricate interplay of solvent quality (polymer-solvent interactions) and solvent strength (polymer-surface vs. solvent-surface interactions). Increasing grafting density and length of grafts protect the backbone against adsorption, but the behavior is non-trivial. A decrease in solvent quality promotes the adsorption, because it lowers the overall solubility, but the backbone collapses and the probability of backbone-surface contacts decreases, which simultaneously hinders the adsorption. The results of simulations are presented in the form of phase diagrams depicting the decisive features of the conformational and sorption behavior.

Accession Number: WOS:000429280100054

PubMed ID: 29446424

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Limpouchova, Zuzana	C-7791-2013	0000-0002-2290-1358

ISSN: 1463-9076
eISSN: 1463-9084

Record 156 of 214

Title: Exploration of Enzyme Diversity by Integrating Bioinformatics with Expression Analysis and Biochemical Characterization

Author(s): Vanacek, P (Vanacek, Pavel); Sebestova, E (Sebestova, Eva); Babkova, P (Babkova, Petra); Bidmanova, S (Bidmanova, Sarka); Daniel, L (Daniel, Lukas); Dvorak, P (Dvorak, Pavel); Stepankova, V (Stepankova, Veronika); Chaloupkova, R (Chaloupkova, Radka); Brezovsky, J (Brezovsky, Jan); Prokop, Z (Prokop, Zbynek); Damborsky, J (Damborsky, Jiri)

Source: ACS CATALYSIS **Volume:** 8 **Issue:** 3 **Pages:** 2402-2412 **DOI:** 10.1021/acscatal.7b03523 **Published:** MAR 2018

Abstract: Millions of protein sequences are being discovered at an incredible pace, representing an inexhaustible source of biocatalysts. Here, we describe an integrated system for automated in silico screening and systematic characterization of diverse family members. The workflow consists of (i) identification and computational characterization of relevant genes by sequence/structural bioinformatics, (ii) expression analysis and activity screening of selected proteins, and (iii) complete biochemical/biophysical characterization and was validated against the haloalkane dehalogenase family. The sequence-based search identified 658 potential dehalogenases. The subsequent structural bioinformatics prioritized and selected 20 candidates for exploration of protein functional diversity. Out of these 20, the expression analysis and the robotic screening of enzymatic activity provided 8 soluble proteins with dehalogenase activity. The enzymes discovered originated from genetically unrelated Bacteria, Eukaryota, and also Archaea. Overall, the integrated system provided biocatalysts with broad catalytic diversity showing unique substrate specificity profiles, covering a wide range of optimal operational temperature from 20 to 70 degrees C and an unusually broad pH range from 5.7 to 10. We obtained the most catalytically proficient native haloalkane dehalogenase enzyme to date (k(cat)/K-0.5 = 96.8 mM(-1) s(-1)) the most thermostable enzyme with melting temperature 71 degrees C, three different cold-adapted enzymes showing dehalogenase activity at near-to-zero temperatures, and a biocatalyst degrading the warfare chemical sulfur mustard. The established strategy can be adapted to other enzyme families for exploration of their biocatalytic diversity in a large sequence space continuously growing due to the use of next-generation sequencing technologies.

Accession Number: WOS:000426804100087

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Dvorak, Pavel		0000-0002-3215-4763

ISSN: 2155-5435

Record 157 of 214

Title: Cyclic water-trimer encapsulation into D-2(22)-C-84 fullerene

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

Source: CHEMICAL PHYSICS LETTERS **Volume:** 695 **Pages:** 245-248 **DOI:** 10.1016/j.cplett.2018.02.006 **Published:** MAR 2018

Abstract: The cyclic water-trimer encapsulations into D-2(22)-C-84 fullerene are evaluated. The encapsulation energy is computed at the M06-2X/6-31++ G** level and it is found that the trimer storage in C-84 yields the potential-energy gain of 10.4 kcal/mol. The encapsulated trimer can have two different forms, either the conformation known with the free gas-phase water trimer or the arrangement with the three nonhydrogen bonded H atoms on the same side of the O-O-O plane. The latter endohedral isomer is lower in the potential energy by 0.071 kcal/mol and forms about 57% of their equilibrium mixture at room temperature. (C) 2018 Elsevier B. V. All rights reserved.

Accession Number: WOS:000427386500039

Author Identifiers:

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

ISSN: 0009-2614
eISSN: 1873-4448

Record 158 of 214

Title: Topological antiferromagnetic spintronics

Author(s): Smejkal, L (Smejkal, Libor); Mokrousov, Y (Mokrousov, Yuriy); Yan, BH (Yan, Binghai); MacDonald, AH (MacDonald, Allan H.)

Source: NATURE PHYSICS **Volume:** 14 **Issue:** 3 **Pages:** 242-251 **DOI:** 10.1038/s41567-018-0064-5 **Published:** MAR 2018

Abstract: The recent demonstrations of electrical manipulation and detection of antiferromagnetic spins have opened up a new chapter in the story of spintronics. Here, we review the emerging research field that is exploring the links between antiferromagnetic spintronics and topological structures in real and momentum space. Active topics include proposals to realize Majorana fermions in antiferromagnetic topological superconductors, to control topological protection and Dirac points by manipulating antiferromagnetic order parameters,

and to exploit the anomalous and topological Hall effects of zero-net-moment antiferromagnets. We explain the basic concepts behind these proposals, and discuss potential applications of topological antiferromagnetic spintronics.
Accession Number: WOS:000426546300013
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Yan, Binghai	D-2404-2013	0000-0003-2164-5839
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Record 159 of 214
Title: Dutch Resolution of a configurationally stable [5]helquat
Author(s): Severa, L (Severa, Lukas); Sazelova, P (Sazelova, Petra); Cisarova, I (Cisarova, Ivana); Saman, D (Saman, David); Koval, D (Koval, Dusan); Devadig, P (Devadig, Pradeep); Kasicka, V (Kasicka, Vaclav); Teply, F (Teply, Filip)
Source: CHIRALITY **Volume:** 30 **Issue:** 3 **Pages:** 254-260 **DOI:** 10.1002/chir.22789 **Published:** MAR 2018
Abstract: Synthesis and nontrivial optical resolution of a helicene-like dication, helquat 1, has been accomplished. Starting with gram scale of the racemic helquat 1 sample, Dutch Resolution using family of 3 tartrate anions was key to achieve successful separation of M and P helical enantiomers of 1. Hundreds of milligrams of each enantiomer of this configurationally stable C-2-symmetric helquat have been obtained. Racemization barrier of 1 has been determined. To our knowledge this is the first report on Dutch Resolution performed with a helicene-like compound. Moreover, there are no literature precedents for Dutch Resolution of chiral quaternary ammonium cations.
Accession Number: WOS:000424886400005
PubMed ID: 29293281
ISSN: 0899-0042
eISSN: 1520-636X

Record 160 of 214
Title: Stable electron beams from laser wakefield acceleration with few-terawatt driver using a supersonic air jet
Author(s): Bohacek, K (Bohacek, K.); Kozlova, M (Kozlova, M.); Nejdl, J (Nejdl, J.); Chaulagain, U (Chaulagain, U.); Horny, V (Horny, V.); Krus, M (Krus, M.); Phuoc, KT (Phuoc, K. Ta)
Source: NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT **Volume:** 883 **Pages:** 24-28 **DOI:** 10.1016/j.nima.2017.11.022 **Published:** MAR 1 2018
Abstract: The generation of stable electron beams produced by the laser wakefield acceleration mechanism with a few-terawatt laser system (600 mJ, 50 fs) in a supersonic synthetic air jet is reported and the requirements necessary to build such a stable electron source are experimentally investigated in conditions near the bubble regime threshold. The resulting electron beams have stable energies of (17.4 +/- 1.1) MeV and an energy spread of (13.5 +/- 1.5) MeV (FWHM), which has been achieved by optimizing the properties of the supersonic gas jet target for the given laser system. Due to the availability of few-terawatt laser systems in many laboratories around the world these stable electron beams open possibilities for applications of this type of particle source. (C) 2017 Elsevier B.V. All rights reserved.
Accession Number: WOS:000419216800005
Author Identifiers:

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Michaela, Kozlova	G-5818-2014	
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Nejdl, Jaroslav	G-5995-2014	0000-0003-0864-8592

ISSN: 0168-9002
eISSN: 1872-9576

Record 161 of 214
Title: Electronic properties of Pu19Os simulating beta-Pu: the strongly correlated Pu phase
Author(s): Havela, L (Havela, L.); Maskova, S (Maskova, S.); Kolorenc, J (Kolorenc, J.); Colineau, E (Colineau, E.); Griveau, JC (Griveau, J-C); Eloirdi, R (Eloirdi, R.)
Source: JOURNAL OF PHYSICS-CONDENSED MATTER **Volume:** 30 **Issue:** 8 **Article Number:** 085601 **DOI:** 10.1088/1361-648X/aaa520 **Published:** FEB 28 2018
Abstract: We established the basic electronic properties of zeta-Pu19Os, which is a close analogue to beta-Pu, and its low-temperature variety, eta-Pu19Os. Their magnetic susceptibility is 15% higher than for delta-Pu. A specific heat study of zeta-Pu19Os shows a soft lattice similar to delta-Pu, leading to a low Debye temperature Theta(D) = 101 K. The linear electronic coefficient gamma related to the quasiparticle density of states at the Fermi level points to a higher value, 55 +/- 2 mJ (mol Pu K-2)(-1), compared to 40 mJ (mol K-2)(-1) for delta-Pu. The results confirm that beta-Pu is probably the most strongly correlated Pu phase, as had been indicated by resistivity measurements. The volume and related Pu-Pu spacing is clearly not the primary tuning parameter for Pu metal, as the beta-Pu density stands close to the ground-state alpha-phase and is much higher than that for delta-Pu. The eta-Pu19Os phase has a record gamma-value of 74 +/- 2 mJ (mol Pu K-2)(-1). The enhancement is not reproduced by LDA+DMFT calculations in the fcc structure, which suggests that multiple diverse sites can be the key to the understanding of beta-Pu.
Accession Number: WOS:000424018100001
PubMed ID: 29388557
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302
Maskova, Silvie	P-4172-2017	0000-0002-0154-7951
Havela, Ladislav		0000-0001-9801-7094

ISSN: 0953-8984
eISSN: 1361-648X

Record 162 of 214
Title: Flavin Photocatalysts for Visible-Light [2+2] Cycloadditions: Structure, Reactivity and Reaction Mechanism
Author(s): Mojr, V (Mojr, Viktor); Pitrova, G (Pitrova, Gabriela); Strakova, K (Strakova, Karolina); Prukala, D (Prukala, Dorota); Brazevic, S (Brazevic, Sabina); Svobodova, E (Svobodova, Eva); Hoskovcova, I (Hoskovcova, Irena); Burdzinski, G (Burdzinski, Gotard); Slanina, T (Slanina, Tomas); Sikorski, M (Sikorski, Marek); Cibulka, R (Cibulka, Radek)
Source: CHEMCATCHEM **Volume:** 10 **Issue:** 4 **Pages:** 849-858 **DOI:** 10.1002/cctc.201701490 **Published:** FEB 21 2018
Abstract: New photocatalysts from the flavin family were found to mediate the [2+2] photocycloaddition reaction. 3-Butyl-10-methyl-5-deazaflavin (3a) and 1-butyl-7,8-dimethoxy-3-methylalloxazine (2e), if irradiated by visible light, were shown to allow an efficient (Phi approximate to 3-10%) intramolecular cyclisation of various types of substrates including substituted styrene dienes and bis(aryl enones), considered as electron-rich and electron-poor substrates, respectively, without any additional reagent. The versatility of the procedure was demonstrated by the cyclisation of photosensitive cinnamyl (E)-3-iodoallyl ether. Structure-activity studies found alloxazine 2e was more active than 7-monosubstituted (R = Cl, Br and MeO) alloxazines. The introduction of chlorine and bromine atom on the deazaflavin skeleton did not enhance the catalytic efficiency of 3a. A detailed electrochemical and spectroscopic study explains the reaction mechanism proceeding through energy transfer from the flavin excited triplet state to the diene followed by its cyclisation.
Accession Number: WOS:000425626700026
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Slanina, Tomas	B-5598-2018	0000-0001-8092-7268
Cibulka, Radek	H-1298-2016	0000-0002-8584-7715
Sikorski, Marek	A-8102-2008	0000-0002-9527-7322
Mojr, Viktor		0000-0002-7543-4087

ISSN: 1867-3880

eISSN: 1867-3899

Record 163 of 214

Title: Dual in vitro and in silico analysis of thiacalix[4]arene dinaphthalene sulfonate for the sensing of 4-nitrotoluene and 2,3-dinitrotoluene

Author(s): Modi, K (Modi, Krunal); Panchal, U (Panchal, Urvi); Patel, C (Patel, Chirag); Bhatt, K (Bhatt, Keyur); Dey, S (Dey, Shuvankar); Mishra, D (Mishra, Divya); Jain, VK (Jain, V. K.)

Source: NEW JOURNAL OF CHEMISTRY **Volume:** 42 **Issue:** 4 **Pages:** 2682-2691 **DOI:** 10.1039/c7nj03820h **Published:** FEB 21 2018

Abstract: A new fluorescent thiacalix[4]arene dinaphthalene sulfonate (TCDNS) was synthesized by a reaction of thiacalix[4]arene with naphthalene sulfonyl chloride. TCDNS was characterized by 1H-NMR, 13C-NMR, and ESI-MS spectrometric analyses. The selectivity of fluoroionophore was analyzed for 4-nitrotoluene (4-NT) and 2,3-dinitrotoluene (2,3-DNT) among various nitroaromatic compounds (NACs) using the spectrofluorimetric technique. 4-NT and 2,3-DNT behave as the strong emission quenchers for TCDNS. The information about the complexation of TCDNS with 4-NT and 2,3-DNT was revealed by ESI-MS and 1H NMR analysis. A standard addition method was used for the detection of 4-NT and 2,3-DNT in a water sample. The complex formation in the cases of TCDNS superset of 4-NT and TCDNS superset of 2,3-DNT has been demonstrated by molecular docking and dynamics simulation techniques.

Accession Number: WOS:000424970300040

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Modi, Krunal	G-1015-2016	0000-0002-1151-1207
Patel, Chirag		0000-0003-0777-7720

ISSN: 1144-0546
eISSN: 1369-9261

Record 164 of 214

Title: Cobalt adatoms on graphene: Effects of anisotropies on the correlated electronic structure

Author(s): Mozara, R (Mozara, R.); Valentyuk, M (Valentyuk, M.); Krivenko, I (Krivenko, I.); Sasioglu, E (Sasioglu, E.); Kolorenc, J (Kolorenc, J.); Lichtenstein, AI (Lichtenstein, A. I.)

Source: PHYSICAL REVIEW B **Volume:** 97 **Issue:** 8 **Article Number:** 085133 **DOI:** 10.1103/PhysRevB.97.085133 **Published:** FEB 20 2018

Abstract: Impurities on surfaces experience a geometric symmetry breaking induced not only by the on-site crystal-field splitting and the orbital-dependent hybridization, but also by different screening of the Coulomb interaction in different directions. We present a many-body study of the Anderson impurity model representing a Co adatom on graphene, taking into account all anisotropies of the effective Coulomb interaction, which we obtained by the constrained random-phase approximation. The most pronounced differences are naturally displayed by the many-body self-energy projected onto the single-particle states. For the solution of the Anderson impurity model and analytical continuation of the Matsubara data, we employed new implementations of the continuous-time hybridization expansion quantum Monte Carlo and the stochastic optimization method, and we verified the results in parallel with the exact diagonalization method.

Accession Number: WOS:000425493000005

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302

ISSN: 2469-9950
eISSN: 2469-9969

Record 165 of 214

Title: Redescription of Paradiplozoon hemiculteri (Monogenea, Diplozoidae) from the type host Hemiculter leucisculus, with neotype designation

Author(s): Jirsova, D (Jirsova, Dagmar); Ding, XJ (Ding, Xuejuan); Civanova, K (Civanova, Kristina); Jirounkova, E (Jirounkova, Eliska); Ilgova, J (Ilgova, Jana); Koubkova, B (Koubkova, Bozena); Kasny, M (Kasny, Martin); Gelnar, M (Gelnar, Milan)

Source: PARASITE **Volume:** 25 **Article Number:** 4 **DOI:** 10.1051/parasite/2018004 **Published:** FEB 9 2018

Abstract: Paradiplozoon hemiculteri (Ling, 1973), a member of the Diplozoidae, parasitizes the gills of Asian fish. Not only is the type material unavailable for this species, the original description was poor and somewhat conflicting, and adequate molecular data were not available. What is more, the available morphological and molecular data are inconsistent and fluctuate significantly. Here, we present a redescription of P. hemiculteri based on morphological and molecular data from new isolates collected from the type host, the sharpbelly Hemiculter leucisculus (Basilewsky, 1855), captured at the neotype locality (Shaoguan, Guangdong Province, southern China); a neotype for P. hemiculteri was designated from this collection. The length and width of the body, buccal suckers, pharynx, attachment clamps, sickle and the central hook handle were all measured and the shape of the anterior and posterior part of the median plate and anterior and posterior joining sclerites accurately documented. Phylogenetic analyses based on the sequences of the second rDNA internal transcribed spacer (ITS2) indicated that all new samples clustered together and differed clearly from sequences attributed to P. hemiculteri, which are deposited in GenBank. Our results confirm that P. hemiculteri is the only diplozoid that has demonstrably been found on the gills of H. leucisculus to date.

Accession Number: WOS:000425084100001

PubMed ID: 29424339

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Civanova, Kristina	G-1182-2014	

ISSN: 1252-607X
eISSN: 1776-1042

Record 166 of 214

Title: Redox Potentials for Tetraplatin, Satraplatin, Its Derivatives, and Ascorbic Acid: A Computational Study

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

Source: INORGANIC CHEMISTRY **Volume:** 57 **Issue:** 3 **Pages:** 951-962 **DOI:** 10.1021/acs.inorgchem.7b01894 **Published:** FEB 5 2018

Abstract: Redox potentials of the Pt(IV) complexes, such as satraplatin, tetraplatin, and several others, are determined at the density functional theory (DFT) level (with B3LYP, omega-B97XD, PBE1PBE, TPSSTPSS, M06-L, M11-L, and MN12-L functionals) and compared with post-Hartree-Fock methods MP2 and CCSD(T). Calculations are performed in water solution employing an implicit solvation model. The impact of replacement of a chloro ligand by a water molecule (hydration in the equatorial plane of the complexes) is also explored. Furthermore, an influence of solvent pH on the magnitude of the redox potentials is discussed for such hydrated complexes. The obtained results are compared with available experimental data leading to a root-mean-square deviation (RMSD) of ca. 0.23 V, using the CCSD(T)/6-31+G(d)/IEF-PCM/scaled-UAKS level. Distribution of the electron density is analyzed at the B3LYP/6-311++G(2df,2pd) level. Also, a correlation between binding energies of axial ligands and the redox potential is demonstrated. Since the Pt(IV) complexes are considered in the framework of anticancer treatment, possible reducing agents in bioenvironment are searched. From this reason, the reduction potential of different protonation states of ascorbic acid is also presented.

Accession Number: WOS:000424730800010

PubMed ID: 29363964

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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ISSN: 0020-1669
eISSN: 1520-510X

Record 167 of 214

Title: meso-Octamethylcalix[4]pyrrole as an effective macrocyclic receptor for the univalent thallium cation in the gas phase: 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: JOURNAL OF MOLECULAR STRUCTURE **Volume:** 1153 **Pages:** 78-84 **DOI:** 10.1016/j.molstruc.2017.09.103 **Published:** FEB 5 2018

Abstract: By using electrospray ionization mass spectrometry (ESI-MS), it was proven experimentally that the univalent thallium cation (Tl+) forms with meso-octamethylcalix[4]pyrrole (1) the cationic complex species 1 Tl+. When this kinetically stable cation-pi complex 1 Tl+ is collisionally activated, it decomposes by elimination of the whole ligand 1 or small meso-octamethylcalix[4]pyrrole fragments. Further, applying quantum chemical DFT calculations, four different conformations of the resulting complex I Tl+

were derived. It means that under the present experimental conditions, this ligand 1 can be considered as a very effective macrocyclic receptor for the thallium cation. (C) 2017 Elsevier B.V. All rights reserved.

Accession Number: WOS:000416191800011

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Polasek, Miroslav	G-7217-2014	

ISSN: 0022-2860

eISSN: 1872-8014

Record 168 of 214

Title: Poly-N-Acetyllactosamine Neo-Glycoproteins as Nanomolar Ligands of Human Galectin-3: Binding Kinetics and Modeling

Author(s): Bumba, L (Bumba, Ladislav); Laaf, D (Laaf, Dominic); Spiwok, V (Spiwok, Vojtech); Elling, L (Elling, Lothar); Kren, V (Kren, Vladimir); Bojarova, P (Bojarova, Pavla)

Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES **Volume:** 19 **Issue:** 2 **Article Number:** 372 **DOI:** 10.3390/ijms19020372 **Published:** FEB 2018

Abstract: Galectin-3 (Gal-3) is recognized as a prognostic marker in several cancer types. Its involvement in tumor development and proliferation makes this lectin a promising target for early cancer diagnosis and anti-cancer therapies. Gal-3 recognizes poly-N-acetyllactosamine (LacNAc)-based carbohydrate motifs of glycoproteins and glycolipids with a high specificity for internal LacNAc epitopes. This study analyzes the mode and kinetics of binding of Gal-3 to a series of multivalent neo-glycoproteins presenting complex poly-LacNAc-based oligosaccharide ligands on a scaffold of bovine serum albumin. These neo-glycoproteins rank among the strongest Gal-3 ligands reported, with K-d reaching sub-nanomolar values as determined by surface plasmon resonance. Significant differences in the binding kinetics were observed within the ligand series, showing the tetrasaccharide capped with N,N-diacetyllactosamine (LacdiNAc) as the strongest ligand of Gal-3 in this study. A molecular model of the Gal-3 carbohydrate recognition domain with docked oligosaccharide ligands is presented that shows the relations in the binding site at the molecular level. The neo-glycoproteins presented herein may be applied for selective recognition of Gal-3 both on the cell surface and in blood serum.

Accession Number: WOS:000427527400056

PubMed ID: 29373511

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Elling, Lothar	B-3711-2013	0000-0002-3654-0397
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Spiwok, Vojtech	A-7747-2008	0000-0001-8108-2033
Bumba, Ladislav	H-2494-2014	
Bumba, Ladislav		0000-0001-6659-5447

ISSN: 1422-0067

Record 169 of 214

Title: Approximating maxmin strategies in imperfect recall games using A-loss recall property

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

Source: INTERNATIONAL JOURNAL OF APPROXIMATE REASONING **Volume:** 93 **Pages:** 290-326 **DOI:** 10.1016/j.ijar.2017.11.010 **Published:** FEB 2018

Abstract: Extensive-form games with imperfect recall are an important model of dynamic games where the players are allowed to forget previously known information. Often, imperfect recall games result from an abstraction algorithm that simplifies a large game with perfect recall. Solving imperfect recall games is known to be a hard problem, and thus it is useful to search for a subclass of imperfect recall games which offers sufficient memory savings while being efficiently solvable. The abstraction process can then be guided to result in a game from this class. We focus on a subclass of imperfect recall games called A-loss recall games. First, we provide a complete picture of the complexity of solving imperfect recall and A-loss recall games. We show that the A-loss recall property allows us to compute a best response in polynomial time (computing a best response is NP-hard in imperfect recall games). This allows us to create a practical algorithm for approximating maxmin strategies in two-player games where the maximizing player has imperfect recall and the minimizing player has A-loss recall. This algorithm is capable of solving some games with up to 5.109 states in approximately 1 hour. Finally, we demonstrate that the use of imperfect recall abstraction can reduce the size of the strategy representation to as low as 0.03% of the size of the strategy representation in the original perfect recall game without sacrificing the quality of the maxmin strategy obtained by solving this abstraction. (C) 2017 Elsevier Inc. All rights reserved.

Accession Number: WOS:000424721400017

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Author	ResearcherID Number	ORCID Number
Lisy, Viliam		0000-0002-1647-1507

ISSN: 0888-613X

eISSN: 1873-4731

Record 170 of 214

Title: P4-To-VHDL: Automatic generation of high-speed input and output network blocks

Author(s): Benacek, P (Benacek, Pavel); Pus, V (Pus, Viktor); Kubatova, H (Kubatova, Hana); Cejka, T (Cejka, Tomas)

Source: MICROPROCESSORS AND MICROSYSTEMS **Volume:** 56 **Pages:** 22-33 **DOI:** 10.1016/j.micpro.2017.10.012 **Published:** FEB 2018

Abstract: High-performance embedded architectures typically contain many stand-alone blocks which communicate and exchange data; additionally a high-speed network interface is usually needed at the boundary of the system. The software-based data processing is typically slow which leads to a need for hardware accelerated approaches. The problem is getting harder if the supported protocol stack is rapidly changing. Such problem can be effectively solved by the Field Programmable Gate Arrays and high-level synthesis which together provide a high degree of generality. This approach has several advantages like fast development or possibility to enable the area of packet-oriented communication to domain oriented experts. However, the typical. disadvantage of this approach is the insufficient performance of generated system from a high-level description. This can be a serious problem in the case of a system which is required to process data at high packet rates. This work presents a generator of high-speed input (Parser) and output (Deparser) network blocks from the P4 language which is designed for the description of modern packet processing devices. The tool converts a P4 description to a synthesizable VHDL code suitable for the FPGA implementation. We present design, analysis and experimental results of our generator. Our results show that the generated circuits are able to process 100 Gbps traffic with fairly complex protocol structure at line rate on Xilinx Virtex-7 XCVH580T FPGA. The approach can be used not only in networking devices but also in other applications like packet processing engines in embedded cores because the P4 language is device and protocol independent.

Accession Number: WOS:000423641500003

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Author	ResearcherID Number	ORCID Number
Cejka, Tomas		0000-0001-7794-9511

ISSN: 0141-9331

eISSN: 1872-9436

Record 171 of 214

Title: Optoelectronic Structure and Related Transport Properties of Ag2Sb2O6 and Cd2Sb2O7

Author(s): Irfan, M (Irfan, Muhammad); Hussain, S (Hussain, Safdar); Khan, SA (Khan, Saleem Ayaz); Goumri-Said, S (Goumri-Said, Souraya); Azam, S (Azam, Sikander)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 47 **Issue:** 2 **Pages:** 1481-1489 **DOI:** 10.1007/s11664-017-5939-1 **Published:** FEB 2018

Abstract: Using the full-potential linearized augmented-plane wave method, the electronic structure and thermoelectric properties of Ag2Sb2O6 and Cd2Sb2O7 compounds have been explored. The modified Becke-Johnson potential was applied to treat the exchange-correlation energy term. The electronic band structures reveal that the valence-band maximum and conduction-band minimum occur at C point, indicating that Ag2Sb2O6 and Cd2Sb2O7 are direct energy bandgap semiconductors. Strong hybridization appeared between Ag (Cd)-s/p and O-s/p states. The optical properties, i.e., complex dielectric function, reflectivity, refractive index, and energy loss function, reveal high reflectivity in the ultraviolet energy range, indicating usefulness of these materials in shields from high-energy radiation. Combining transport theory and the outputs from the full-potential linearized augmented-plane wave calculations, the thermoelectric properties were analyzed as functions of temperature. Due to their high thermopower and narrow bandgap, Ag2Sb2O6 and Cd2Sb2O7 are suitable materials for application in optoelectronic and thermoelectric devices.

Accession Number: WOS:000419791800072

Record 172 of 214
Title: Gas adsorption and dynamics in Pillared Graphene Frameworks
Author(s): Pedrielli, A (Pedrielli, Andrea); Taioli, S (Taioli, Simone); Garberoglio, G (Garberoglio, Giovanni); Pugno, NM (Pugno, Nicola Maria)
Source: MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 257 **Pages:** 222-231 **DOI:** 10.1016/j.micromeso.2017.08.034 **Published:** FEB 2018
Abstract: Pillared Graphene Frameworks are a novel class of microporous materials made by graphene sheets separated by organic spacers. One of their main features is that the pillar type and density can be chosen to tune the material properties. In this work, we present a computer simulation study of adsorption and dynamics of H-2, CH4, CO2, N-2 and O-2 and binary mixtures thereof, in Pillared Graphene Frameworks with nitrogen-containing organic spacers. In general, we find that pillar density plays the most important role in determining gas adsorption. In the low-pressure regime (<= 10 bar) the amount of gas adsorbed is an increasing function of pillar density. At higher pressure the opposite trend is observed. Diffusion coefficients were computed for representative structures taking into account the framework flexibility that is essential for assessing the dynamical properties of the adsorbed gases. Good performance for the gas separation in CH4/H-2, CO2/F-2 and CO2/N-2 mixtures was found, with values comparable to those of metal organic frameworks and zeolites. (C) 2017 Elsevier Inc. All rights reserved.
Accession Number: WOS:000418106600025
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Garberoglio, Giovanni		0000-0002-9201-2716

Record 173 of 214
Title: Rotation invariants of vector fields from orthogonal moments
Author(s): Yang, B (Yang, Bo); Kostkova, J (Kostkova, Jitka); Flusser, J (Flusser, Jan); Suk, T (Suk, Tomas); Bujack, R (Bujack, Roxana)
Source: PATTERN RECOGNITION **Volume:** 74 **Pages:** 110-121 **DOI:** 10.1016/j.patcog.2017.09.004 **Published:** FEB 2018
Abstract: Vector field images are a type of new multidimensional data that appear in many engineering areas. Although the vector fields can be visualized as images, they differ from graylevel and color images in several aspects. To analyze them, special methods and algorithms must be originally developed or substantially adapted from the traditional image processing area. In this paper, we propose a method for the description and matching of vector field patterns under an unknown rotation of the field. Rotation of a vector field is so-called total rotation, where the action is applied not only on the spatial coordinates but also on the field values. Invariants of vector fields with respect to total rotation constructed from orthogonal Gaussian Hermite moments and Zernike moments are introduced. Their numerical stability is shown to be better than that of the invariants published so far. We demonstrate their usefulness in a real world template matching application of rotated vector fields. (C) 2017 Published by Elsevier Ltd.
Accession Number: WOS:000417547800009
Author Identifiers:

Author	ResearcherID Number	ORCID Number
, Jan		0000-0003-3747-9214

Record 174 of 214
Title: Modeling of inhomogeneous mixing of plasma species in argon-steam arc discharge
Author(s): Jenista, J (Jenista, J.); Takana, H (Takana, H.); Uehara, S (Uehara, S.); Nishiyama, H (Nishiyama, H.); Bartlova, M (Bartlova, M.); Aubrecht, V (Aubrecht, V.); Murphy, AB (Murphy, A. B.)
Source: JOURNAL OF PHYSICS D-APPLIED PHYSICS **Volume:** 51 **Issue:** 4 **Article Number:** 045202 **DOI:** 10.1088/1361-6463/aa9f6f **Published:** JAN 31 2018
Abstract: This paper presents numerical simulation of mixing of argon- and water-plasma species in an argon- steam arc discharge generated in a thermal plasma generator with the combined stabilization of arc by axial gas flow (argon) and water vortex. The diffusion of plasma species itself is described by the combined diffusion coefficients method in which the coefficients describe the diffusion of argon 'gas,' with respect to water vapor 'gas.' Diffusion processes due to the gradients of mass density, temperature, pressure, and an electric field have been considered in the model. Calculations for currents 150-400 A with 15-22.5 standard liters per minute (slm) of argon reveal inhomogeneous mixing of argon and oxygen-hydrogen species with the argon species prevailing near the arc axis. All the combined diffusion coefficients exhibit highly nonlinear distribution of their values within the discharge, depending on the temperature, pressure, and argon mass fraction of the plasma. The argon diffusion mass flux is driven mainly by the concentration and temperature space gradients. Diffusions due to pressure gradients and due to the electric field are of about 1 order lower. Comparison with our former calculations based on the homogeneous mixing assumption shows differences in temperature, enthalpy, radiation losses, arc efficiency, and velocity at 400 A. Comparison with available experiments exhibits very good qualitative and quantitative agreement for the radial temperature and velocity profiles 2 mm downstream of the exit nozzle.
Accession Number: WOS:000419800200001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Murphy, Anthony	A-7796-2008	0000-0002-2820-2304
Aubrecht, Vladimir	C-3482-2008	0000-0002-1380-4169
Jenista, Jiri	H-2278-2014	
Bartlova, Milada		0000-0002-3888-8493

Record 175 of 214
Title: Aggregate Size Dependence of Amyloid Adsorption onto Charged Interfaces
Author(s): Tesei, G (Tesei, Giulio); Hellstrand, E (Hellstrand, Erik); Sanagavarapu, K (Sanagavarapu, Kalyani); Linse, S (Linse, Sara); Sparr, E (Sparr, Emma); Vacha, R (Vacha, Robert); Lund, M (Lund, Mikael)
Source: LANGMUIR **Volume:** 34 **Issue:** 4 **Pages:** 1266-1273 **DOI:** 10.1021/acs.langmuir.7b03155 **Published:** JAN 30 2018
Abstract: Amyloid aggregates are associated with a range of human neuro-degenerative disorders, and it has been shown that neurotoxicity is dependent on aggregate size. Combining molecular simulation with analytical theory, a predictive model is proposed for the adsorption of amyloid aggregates onto oppositely charged surfaces, where the interaction is governed by an interplay between electrostatic attraction and entropic repulsion. Predictions are experimentally validated against quartz crystal microbalance-dissipation experiments of amyloid beta peptides and fragmented fibrils in the presence of a supported lipid bilayer. Assuming amyloids as rigid, elongated particles, we observe nonmonotonic trends for the extent of adsorption with respect to aggregate size and preferential adsorption of smaller aggregates over larger ones. Our findings describe a general phenomenon with implications for stiff polyions and rodlike particles that are electrostatically attracted to a surface.
Accession Number: WOS:000424070400005
PubMed ID: 29284092
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Tesei, Giulio		0000-0003-4339-4460

Record 176 of 214
Title: Structure of tick-borne encephalitis virus and its neutralization by a monoclonal antibody
Author(s): Fuzik, T (Fuzik, Tibor); Formanova, P (Formanova, Petra); Ruzek, D (Ruzek, Daniel); Yoshii, K (Yoshii, Kentaro); Niedrig, M (Niedrig, Matthias); Plevka, P (Plevka, Pavel)
Source: NATURE COMMUNICATIONS **Volume:** 9 **Article Number:** 436 **DOI:** 10.1038/s41467-018-02882-0 **Published:** JAN 30 2018

Abstract: Tick-borne encephalitis virus (TBEV) causes 13,000 cases of human meningitis and encephalitis annually. However, the structure of the TBEV virion and its interactions with antibodies are unknown. Here, we present cryo-EM structures of the native TBEV virion and its complex with Fab fragments of neutralizing antibody 19/1786. Flavivirus genome delivery depends on membrane fusion that is triggered at low pH. The virion structure indicates that the repulsive interactions of histidine side chains, which become protonated at low pH, may contribute to the disruption of heterotetramers of the TBEV envelope and membrane proteins and induce detachment of the envelope protein ectodomains from the virus membrane. The Fab fragments bind to 120 out of the 180 envelope glycoproteins of the TBEV virion. Unlike most of the previously studied flavivirus-neutralizing antibodies, the Fab fragments do not lock the E-proteins in the native-like arrangement, but interfere with the process of virus-induced membrane fusion.
Accession Number: WOS:000423510600013
PubMed ID: 29382836
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Ruzek, Daniel	G-9275-2014	0000-0003-4655-2380
Plevka, Pavel	H-8661-2014	0000-0003-4215-3315

ISSN: 2041-1723

Record 177 of 214
Title: Radiative decay of HeLi+(b(3)Sigma(+))
Author(s): Zamecnikova, M (Zamecnikova, Martina); Soldan, P (Soldan, Pavel)
Source: CHEMICAL PHYSICS **Volume:** 500 **Pages:** 1-6 **DOI:** 10.1016/j.chemphys.2017.11.001 **Published:** JAN 26 2018
Abstract: Radiative lifetimes of the ro-vibrational bound states of HeLi+(b(3)Sigma(+)) are calculated quantum-mechanically when both bound-bound and bound-free processes are taken into account. The calculations are restricted to the initial states with low rotational quantum numbers. For the rotationless molecular ion, the shortest lifetime is 1.30×10^{-6} s of the ground vibrational state. With increasing vibration excitations the radiative lifetimes slightly increase, but keep below 10^{-5} s for the next 17 vibrational states, then they start to increase more rapidly up to 2.41×10^{-2} s for the highest vibrational state. The radiative lifetimes also tend to slightly prolong with increasing rotational excitations but stay on the same magnitude for the low rotational quantum numbers. (C) 2017 Elsevier B.V. All rights reserved.
Accession Number: WOS:000424577300001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
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Soldan, Pavel	C-2256-2008	0000-0002-6281-7599

ISSN: 0301-0104
eISSN: 1873-4421

Record 178 of 214
Title: A critical comparison of topology-based pathway analysis methods
Author(s): Ihnatova, I (Ihnatova, Ivana); Popovici, V (Popovici, Vlad); Budinska, E (Budinska, Eva)
Source: PLOS ONE **Volume:** 13 **Issue:** 1 **Article Number:** e0191154 **DOI:** 10.1371/journal.pone.0191154 **Published:** JAN 25 2018
Abstract: One of the aims of high-throughput gene/protein profiling experiments is the identification of biological processes altered between two or more conditions. Pathway analysis is an umbrella term for a multitude of computational approaches used for this purpose. While in the beginning pathway analysis relied on enrichment-based approaches, a newer generation of methods is now available, exploiting pathway topologies in addition to gene/protein expression levels. However, little effort has been invested in their critical assessment with respect to their performance in different experimental setups. Here, we assessed the performance of seven representative methods identifying differentially expressed pathways between two groups of interest based on gene expression data with prior knowledge of pathway topologies: SPIA, PRS, CePa, TAPPA, TopologyGSA, Clipper and DEGraph. We performed a number of controlled experiments that investigated their sensitivity to sample and pathway size, threshold-based filtering of differentially expressed genes, ability to detect target pathways, ability to exploit the topological information and the sensitivity to different preprocessing strategies. We also verified type I error rates and described the influence of overexpression of single genes, gene sets and topological motifs of various sizes on the detection of a pathway as differentially expressed. The results of our experiments demonstrate a wide variability of the tested methods. We provide a set of recommendations for an informed selection of the proper method for a given data analysis task.
Accession Number: WOS:000423416600042
PubMed ID: 29370226
Author Identifiers:

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Budinska, Eva	F-2698-2011	0000-0002-9004-9187
Popovici, Vlad	C-2039-2008	0000-0002-1311-9188

ISSN: 1932-6203

Record 179 of 214
Title: Large Converse Piezoelectric Effect Measured on a Single Molecule on a Metallic Surface
Author(s): Stetsovych, O (Stetsovych, Oleksandr); Mutombo, P (Mutombo, Pingo); Svec, M (Svec, Martin); Samal, M (Samal, Michal); Nejedly, J (Nejedly, Jindrich); Cisarova, I (Cisarova, Ivana); Vazquez, H (Vazquez, Hector); Moro-Lagares, M (Moro-Lagares, Maria); Berger, J (Berger, Jan); Vacek, J (Vacek, Jaroslav); Stara, IG (Stara, Irena G.); Stary, I (Stary, Ivo); Jelinek, P (Jelinek, Pavel)
Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 140 **Issue:** 3 **Pages:** 940-946 **DOI:** 10.1021/jacs.7b08729 **Published:** JAN 24 2018
Abstract: The converse piezoelectric effect is a phenomenon in which mechanical strain is generated in a material due to an applied electrical field. In this work, we demonstrate the Converse piezoelectric effect in single heptahelicene-derived molecules on the Ag(111) surface using atomic, force microscopy (AFM) and total energy density functional theory (DFT) calculations. The force distance spectroscopy acquired over a wide range of bias voltages reveals a linear shift of the tip sample distance at which the contact between the molecule and tip apex is established. We demonstrate that this effect is caused by the bias-induced deformation of the spring-like scaffold of the helical polyaromatic molecules. We attribute this effect to coupling of a soft vibrational mode of the molecular helix with a vertical electric dipole induced by molecule substrate charge transfer. In addition, we also performed the same spectroscopic measurements on a more rigid o-carborane dithiol molecule on the Ag(111) surface. In this case, we identify a weaker linear electromechanical response, which underpins the importance of the helical scaffold on the observed piezoelectric response.
Accession Number: WOS:000423496700020
PubMed ID: 29275621
Author Identifiers:

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Mutombo, Pingo		0000-0002-8175-7587
Vazquez, Hector		0000-0002-3865-9922

ISSN: 0002-7863

Record 180 of 214
Title: HybPhyloMaker: Target Enrichment Data Analysis From Raw Reads to Species Trees
Author(s): Fer, T (Fer, Tomas); Schmickl, RE (Schmickl, Roswitha E.)
Source: EVOLUTIONARY BIOINFORMATICS **Volume:** 14 **Article Number:** 1176934317742613 **DOI:** 10.1177/1176934317742613 **Published:** JAN 12 2018
Abstract: Hybridization-based target enrichment in combination with genome skimming (Hyb-Seq) is becoming a standard method of phylogenomics. We developed HybPhyloMaker, a bioinformatics pipeline that performs target enrichment data analysis from raw reads to supermatrix-, supertree-, and multispecies coalescent-based species tree reconstruction. HybPhyloMaker is written in BASH and integrates common bioinformatics tools. It can be launched both locally and on a high-performance computer cluster. Compared with existing

target enrichment data analysis pipelines, HybPhyloMaker offers the following main advantages: implementation of all steps of data analysis from raw reads to species tree reconstruction, calculation and summary of alignment and gene tree properties that assist the user in the selection of "quality-filtered" genes, implementation of several species tree reconstruction methods, and analysis of the coding regions of organellar genomes.

Accession Number: WOS:000424039200001
PubMed ID: 29348708
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Schmickl, Roswitha	H-1624-2014	0000-0002-0632-5143

ISSN: 1176-9343

Record 181 of 214
Title: Weakly perturbative imaging of interfacial water with submolecular resolution by atomic force microscopy
Author(s): Peng, JB (Peng, Jinbo); Guo, J (Guo, Jing); Hapala, P (Hapala, Prokop); Cao, DY (Cao, Duanyun); Ma, RZ (Ma, Runze); Cheng, BW (Cheng, Bowei); Xu, LM (Xu, Limei); Ondracek, M (Ondracek, Martin); Jelinek, P (Jelinek, Pavel); Wang, EG (Wang, Enge); Jiang, Y (Jiang, Ying)
Source: NATURE COMMUNICATIONS **Volume:** 9 **Article Number:** 122 **DOI:** 10.1038/s41467-017-02635-5 **Published:** JAN 9 2018

Abstract: Scanning probe microscopy has been extensively applied to probe interfacial water in many interdisciplinary fields but the disturbance of the probes on the hydrogen-bonding structure of water has remained an intractable problem. Here, we report submolecular-resolution imaging of the water clusters on a NaCl(001) surface within the nearly noninvasive region by a qPlus-based noncontact atomic force microscopy. Comparison with theoretical simulations reveals that the key lies in probing the weak high-order electrostatic force between the quadrupole-like CO-terminated tip and the polar water molecules at large tip-water distances. This interaction allows the imaging and structural determination of the weakly bonded water clusters and even of their metastable states with negligible disturbance. This work may open an avenue for studying the intrinsic structure and dynamics of ice or water on surfaces, ion hydration, and biological water with atomic precision.

Accession Number: WOS:000419658100021
PubMed ID: 29317638
Author Identifiers:

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Cao, Duanyun		0000-0002-3989-959X
cheng, bo wei		0000-0001-8234-4226

ISSN: 2041-1723

Record 182 of 214
Title: Measurement of IPTV Qualitative Parameters on EPON/VDSL2 Topology
Author(s): Latal, J (Latal, Jan); Wilcek, Z (Wilcek, Zdenek); Kolar, J (Kolar, Jakub); Vojtech, J (Vojtech, Josef)
Edited by: Plank T
Source: 2018 INTERNATIONAL CONFERENCE ON BROADBAND COMMUNICATIONS FOR NEXT GENERATION NETWORKS AND MULTIMEDIA APPLICATIONS (COBCOM) **Published:** 2018

Abstract: The future of telecommunication networks lies in the area of multimedia services that are offered to end customers. The article discusses the possibilities of deploying IPTV service for a hybrid type of telecommunication topology, which is formed by EPON/VDSL2 systems. The advantage of such topologies is the use of already existing telecommunication network and verification of qualitative features of the distributed IPTV data flows at the same moment. Therefore, the main outputs of this article are the possibilities of distributing data packets by means of multicast or unicast operations. The basic qualitative parameters of the video and data flows (PSNR, MSE, and SSIM) were evaluated with the help of the software tool - MSU Video Quality Measurement Tool.

Accession Number: WOS:000454740700016
Conference Title: 2nd International Conference on Broadband Communications for Next Generation Networks and Multimedia Applications (CoBCom)
Conference Date: JUL 11-13, 2018
Conference Location: Graz Univ Technol, Fac Elect Engn, Graz, AUSTRIA
Conference Sponsors: Graz Univ Technol, IEEE Austria Sect, IEEE, IEEE Austria Chapter, Comp Simulat Technol GmbH, X Test, SPINNER Austria GmbH, Glyn GmBH, Infineon Austria, WKO Steiermark, Austrian Electrotechn Assoc
Conference Host: Graz Univ Technol, Fac Elect Engn
ISBN: 978-1-5386-4157-6

Record 183 of 214
Title: QUANTUM-MECHANICAL STUDY OF MAGNETIC PROPERTIES OF SUPERALLOY NANOCOMPOSITE PHASE Fe2AlTi
Author(s): Slavik, A (Slavik, Anton); Mihalikova, I (Mihalikova, Ivana); Friak, M (Friak, Martin); Vsianska, M (Vsianska, Monika); Sob, M (Sob, Mojmir)
Book Group Author(s): TANGER Ltd
Source: 9TH INTERNATIONAL CONFERENCE ON NANOMATERIALS - RESEARCH & APPLICATION (NANOCON 2017) **Pages:** 63-68 **Published:** 2018

Abstract: The L21-structure Fe2AlTi intermetallic compound is one of the two phases identified in Fe-Al-Ti superalloy nanocomposites. Experimental data related to low-temperature magnetic properties of this Heusler compound indicate that magnetic moment is about 0.1 Bohr magneton per formula unit. In contrast, previous quantum-mechanical calculations predicted Fe2AlTi to have much higher magnetic moment, 0.9 Bohr magneton per formula unit. In order to solve this discrepancy between the theory and experiment we have performed a series of quantum-mechanical fix-spin-moment calculations and compared our results with those for non-magnetic state. It turns out that the total energy of the non-magnetic state is only by 10.73 meV/atom higher than that of the magnetic state. When applying Boltzmann statistics to this very small energy difference we predict that the non-magnetic state appears at non-zero temperatures with significant probabilities (for instance, 22.36 % at T = 100 K) and reduces the overall magnetic moment. As another mechanism lowering the magnetization we studied selected shape deformations, in particular trigonal shearing. Fe2AlTi exhibits a compression-tension asymmetry with respect to these strains and, for example, the strain epsilon=-0.08 destabilizes the spin-polarized state, leaving the non-magnetic state as the only stable one.

Accession Number: WOS:000452823300009
Conference Title: 9th International Conference on Nanomaterials - Research and Application (NANOCON)
Conference Date: OCT 18-20, 2017
Conference Location: Brno, CZECH REPUBLIC
Conference Sponsors: Tanger Ltd, Czech Soc New Mat & Technologies, Reg Ctr Adv Technologies & Mat, CS Clean Solut, Nicolet cz, NenoVision, PTIK Instruments, TESCAN, Amer Elements, ABL&E JASCO, Measurement Techn Moravia, Delong Instruments, Exakt, Schaefer, Zeiss, Renishaw, ChromSpec Spol S R O, RAITH, Testo, Analyt & Measuring & Testing
ISBN: 978-80-87294-81-9

Record 184 of 214
Title: FIRST-PRINCIPLES STUDY OF INTERFACE ENERGIES IN Fe-Al-BASED SUPERALLOY NANOCOMPOSITES
Author(s): Mihalikova, I (Mihalikova, Ivana); Slavik, A (Slavik, Anton); Friak, M (Friak, Martin); Vsianska, M (Vsianska, Monika); Koutna, N (Koutna, Nikola); Holec, D (Holec, David); Sob, M (Sob, Mojmir)
Book Group Author(s): TANGER Ltd
Source: 9TH INTERNATIONAL CONFERENCE ON NANOMATERIALS - RESEARCH & APPLICATION (NANOCON 2017) **Pages:** 69-74 **Published:** 2018

Abstract: Fe-Al-based nanocomposites with a superalloy-type of microstructure constitute a very promising class of materials. They possess a great potential as an alternative to the currently used steel grades in high temperature applications. Intermetallics-containing nanocomposites, such as those with the Fe3Al compound being one of the phases, may open a way towards future automotive and energy-conversion technologies with lower fuel consumption and reduced environmental impact. We employ quantum-mechanical calculations to analyze relations between ordering tendencies of Al atoms in the disordered Fe-18.75at.% Al phase on one hand and thermodynamic, structural and magnetic properties of Fe-Al-based nanocomposites on the other. When comparing supercells modeling disordered Fe-Al phase with different atomic distribution of atoms we find out that the supercell without 1st and 2nd nearest neighbor Al-Al pairs has a lower energy than that mimicking a perfect disorder (a special quasi-random structure, SQS). Further, coherent interfaces with (001), (110) and (1-10) crystallographic orientations between Fe3Al compound and SQS Fe-Al phase have higher energies than those exhibiting atomic distribution without 1st and 2nd nearest neighbor Al-Al pairs.

Accession Number: WOS:000452823300010
Conference Title: 9th International Conference on Nanomaterials - Research and Application (NANOCON)

Conference Date: OCT 18-20, 2017
Conference Location: Brno, CZECH REPUBLIC
Conference Sponsors: Tanger Ltd, Czech Soc New Mat & Technologies, Reg Ctr Adv Technologies & Mat, CS Clean Solut, Nicolet cz, NenoVision, PTIK Instruments, TESCAN, Amer Elements, ABL&E JASCO, Measurement Techn Moravia, Delong Instruments, Exakt, Schaefer, Zeiss, Renishaw, ChromSpec Spol S R O, RAITH, Testo, Analyt & Measuring & Testing
ISBN: 978-80-87294-81-9

Record 185 of 214
Title: Multi-purpose infrastructure for dissemination of precise stable optical frequency
Author(s): Vojtech, J (Vojtech, Josef); Havlis, O (Havlis, Ondrej); Slapak, M (Slapak, Martin); Velc, R (Velc, Radek); Munster, P (Munster, Petr); Horvath, T (Horvath, Tomas); Kundrat, J (Kundrat, Jan); Smotlacha, V (Smotlacha, Vladimir); Hrabina, J (Hrabina, Jan); Cizek, M (Cizek, Martin); Pravdova, L (Pravdova, Lenka); Rerucha, S (Rerucha, Simon); Cip, O (Cip, Ondrej); Slavik, R (Slavik, Radan); Vohnout, R (Vohnout, Rudolf); Radil, J (Radil, Jan); Skoda, P (Skoda, Pavel); Altmannova, L (Altmannova, Lada); Altmann, M (Altmann, Michal); Hazlinsky, M (Hazlinsky, Michal)
Edited by: Strojnik M; Kirk MS
Source: INFRARED REMOTE SENSING AND INSTRUMENTATION XXVI **Book Series:** Proceedings of SPIE **Volume:** 10765 **Article Number:** UNSP 1076507 **DOI:** 10.1117/12.2321333 **Published:** 2018
Abstract: Long distance precise frequency and accurate time transfer methods based on optical fiber links have evolved rapidly in recent years, demonstrating excellent performance. They are attractive both for very high-performance applications and as a secure alternative complement to radio-and satellite-based methods. In this paper, we present development of infrastructure for such transmission containing 700+km of transmission lines, with planned cross border optical frequency connectivity. According to our knowledge, this will be the third such line globally. The infrastructure also shares fibers with existing data transmissions, both amplitude and phase modulated, which poses high demands on mutual isolation and insensitivity to cross talks.
Accession Number: WOS:000453462300005
Conference Title: Annual Conference on Infrared Remote Sensing and Instrumentation XXVI held part of the Annual SPIE Optics + Photonics Meeting
Conference Date: AUG 20-22, 2018
Conference Location: San Diego, CA
Conference Sponsors: SPIE
ISSN: 0277-786X
eISSN: 1996-756X
ISBN: 978-1-5106-2102-2

Record 186 of 214
Title: Automatic voice control system for UAV-based accessories
Author(s): Rezac, F (Rezac, Filip); Safarik, J (Safarik, Jakub); Gresak, E (Gresak, Erik); Jalowiczor, J (Jalowiczor, Jakub); Rozhon, J (Rozhon, Jan)
Edited by: Karlsen RE; Gage DW; Shoemaker CM; Nguyen HG
Source: UNMANNED SYSTEMS TECHNOLOGY XX **Book Series:** Proceedings of SPIE **Volume:** 10640 **Article Number:** UNSP 106400P **DOI:** 10.1117/12.2301242 **Published:** 2018
Abstract: This article deals with the system for voice control of the UAV (Unattended Aerial Vehicle) accessories using the mobile device and an advanced communication platform. The paper provides an overview of projects realized in last period in field of voice-controlled drones and explains the applied approach for automatic speech recognition using hidden markov models. Authors describes also converting speech commands instructions for UAV control and necessary steps in practical testing and optimization of the whole system. The achieved results and conclusions are given in the final chapter of the article in which authors provide their experience gained within the experimental development.
Accession Number: WOS:000453080600019
Conference Title: Conference on Unmanned Systems Technology XX
Conference Date: APR 17-19, 2018
Conference Location: Orlando, FL
Conference Sponsors: SPIE
ISSN: 0277-786X
eISSN: 1996-756X
ISBN: 978-1-5106-1792-6

Record 187 of 214
Title: Estimated Total Albumin in Fresh Urine Samples Based on Correlation Between the Roche Immunoturbidimetric and an In-House HPLC Method
Author(s): Fortova, M (Fortova, Magdalena); Klapkova, E (Klapkova, Eva); Sopko, B (Sopko, Bruno); Prusa, R (Prusa, Richard)
Source: CLINICAL LABORATORY **Volume:** 64 **Issue:** 11-12 **Pages:** 1835-1845 **DOI:** 10.7754/Clin.Lab.2018.180410 **Published:** 2018
Abstract: Background: Many studies have reported higher values of urinary albumin measured by high performance liquid chromatography (HPLC) in comparison with immunochemical methods. The aims of our study were the implementation of the HPLC method for albuminuria, testing the hypothesis about coeluting proteins, comparison of albuminuria assessed by HPLC and immunoturbidimetric (IT) methods in diabetic and non-diabetic patient samples.
Methods: We compared albuminuria assessed by HPLC with albuminuria assessed by the IT method in fresh urine samples of 636 diabetics and 456 non-diabetics. We investigated relationships between albuminuria and blood glycated hemoglobin HbA(1c).
Results: We found significant differences between the parameters of linear regressions between albuminuria determined using HPLC and IT among patients with and without DM, and even between patients with DM type 1 and type 2. We confirmed the underestimation of albuminuria assessed by IT. We did not reveal any significant correlation between blood glycated hemoglobin and any of the parameters derived from albuminuria.
Conclusions: We excluded non-specificity of the HPLC method. Despite of a little bit lower analytical sensitivity of the HPLC method in comparison with IT method the diagnostic sensitivity of HPLC method is higher, because it measures the total albuminuria (immunoreactive plus immuno-unreactive). We developed three formulas (for nondiabetics, for diabetics type 1 and diabetics type 2) for the estimation of the total albuminuria from IT values. We also confirmed that albuminuria and HbA(1c) are independent biomarkers.
Accession Number: WOS:000452882500006
PubMed ID: 30549990
ISSN: 1433-6510

Record 188 of 214
Title: Improvement of the visibility of concealed features in misregistered NIR reflectograms by deep learning
Author(s): Blazek, J (Blazek, Jan); Vlasic, O (Vlasic, Oldrich); Zitova, B (Zitova, Barbara)
Book Group Author(s): IOP
Source: FLORENCE HERI-TECH - THE FUTURE OF HERITAGE SCIENCE AND TECHNOLOGIES **Book Series:** IOP Conference Series-Materials Science and Engineering **Volume:** 364 **Article Number:** UNSP 012058 **DOI:** 10.1088/1757-899X/364/1/012058 **Published:** 2018
Abstract: Features of Old Master paintings hidden under the upper layer of a painting are often studied using NIR reflectograms; however their interpretability can be reduced due to the visible content. In our previous work [3] we described the possibility of increasing the visibility of concealed features in NIR reflectograms from the painting surface. The method output, enhanced NIR reflectogram, is produced by extrapolating the VIS data to a NIR range reflectogram and subtracting it from the acquired data in the NIR spectral subband. As a result, separated information from the NIR domain is obtiained. This method has a severe limitation, because it requires precise image registration of the VIS and NIR spectral bands. This is often hard to achieve, because DSLR cameras or multiple devices with various optical systems are used for data collection, and the mutual spatial relation of the images is often unknown. Thus, in the original form, the algorithm was applicable only for data acquired using special scanners producing spatially registered images (as in [4]). In this work, we present an extension of the previous algorithm inspired by deep learning. The new concept allows processing of images only partially registered with pixel precision; subpixel accuracy is no longer needed. We suggest an extension of neural network input with neighboring pixels and allocation of extra ANN layers for translation compensation. The results are demonstrated on misregistered images captured by DSLR camera in VIS and NIR.
Accession Number: WOS:000452025100058
Conference Title: Conference on Florence Heri-Tech - The Future of Heritage Science and Technologies
Conference Date: MAY 16-18, 2018
Conference Location: Florence, ITALY
Conference Sponsors: Univ Florence
ISSN: 1757-8981

Record 189 of 214

Title: INELASTIC MEAN FREE PATH FROM RAW DATA MEASURED BY LOW-ENERGY ELECTRONS TIME-OF-FLIGHT SPECTROMETER
Author(s): Zouhar, M (Zouhar, M.); Radlicka, T (Radlicka, T.); Oral, M (Oral, M.); Konvalina, I (Konvalina, I.)
Edited by: Mika F; Pokorna Z
Source: RECENT TRENDS IN CHARGED PARTICLE OPTICS AND SURFACE PHYSICS INSTRUMENTATION **Pages:** 86-86 **Published:** 2018
Accession Number: WOS:000450591400034
Conference Title: 16th International Seminar of the Institute-of-Scientific-Instruments-The-Czech-Academy-of-Sciences
Conference Date: JUN 04-08, 2018
Conference Location: Brno, CZECH REPUBLIC
Conference Sponsors: Czech Acad Sci, Inst Sci Instruments
ISBN: 978-80-87441-23-7

Record 190 of 214
Title: A Large-Scale Study on Source Code Reviewer Recommendation
Author(s): Lipcak, J (Lipcak, Jakub); Rossi, B (Rossi, Bruno)
Edited by: Bures T; Angelis L
Source: 44TH EUROMICRO CONFERENCE ON SOFTWARE ENGINEERING AND ADVANCED APPLICATIONS (SEAA 2018) **Book Series:** EUROMICRO Conference Proceedings **Pages:** 378-387 **DOI:** 10.1109/SEAA.2018.00068 **Published:** 2018
Abstract: Context: Software code reviews are an important part of the development process, leading to better software quality and reduced overall costs. However, finding appropriate code reviewers is a complex and time-consuming task. Goals: In this paper, we propose a large-scale study to compare performance of two main source code reviewer recommendation algorithms (RevFinder and a Naive Bayes-based approach) in identifying the best code reviewers for opened pull requests. Method: We mined data from Github and Gerrit repositories, building a large dataset of 51 projects, with more than 293K pull requests analyzed, 180K owners and 157K reviewers. Results: Based on the large analysis, we can state that i) no model can be generalized as best for all projects, ii) the usage of a different repository (Gerrit, GitHub) can have impact on the the recommendation results, iii) exploiting sub-projects information available in Gerrit can improve the recommendation results.
Accession Number: WOS:000450238900059
Conference Title: 44th Euromicro Conference on Software Engineering and Advanced Applications (SEAA)
Conference Date: AUG 29-31, 2018
Conference Location: Prague, CZECH REPUBLIC
Conference Sponsors: Czech Tech Univ Prague, Euromicro, CYIENT, ASICentrum, IMA, CESNET, AMCA Conf Agcy
ISSN: 1089-6503
ISBN: 978-1-5386-7383-6

Record 191 of 214
Title: Motion planning of 3D objects using Rapidly Exploring Random Tree guided by approximate solutions
Author(s): Vonasek, V (Vonasek, Vojtech)
Book Group Author(s): IEEE
Source: 2018 IEEE 23RD INTERNATIONAL CONFERENCE ON EMERGING TECHNOLOGIES AND FACTORY AUTOMATION (ETFA) **Book Series:** IEEE International Conference on Emerging Technologies and Factory Automation-ETFA **Pages:** 713-720 **Published:** 2018
Abstract: Path planning of 3D objects, where the task is to find a collision-free path for a rigid 3D object among obstacles, is studied in this paper. This task has many applications mainly in robotics, but also in other fields, e.g., in computer-aided design and computational biology. Sampling-based approaches like Rapidly Exploring Random Trees (RRT) solve the problem by randomized search in the corresponding configuration space. A well known bottleneck of sampling-based methods is the narrow passage problem. Narrow passages are small regions in the configuration space that are difficult to cover by the random samples, which prevents to find a path leading through them. In this paper, we propose a novel extension to Rapidly Exploring Random Tree (RRT) to cope with the narrow passage problem. The proposed planner first solves a simplified (relaxed) version of the problem which is achieved, e.g., by reducing the geometry of the robot. This approximate solution is then used to guide the search in the configuration space for a less relaxed version of the problem, i.e., for a larger robot. The proposed approach is compared to several state-of-the-art path planners in a set of 3D planning benchmarks. Besides, the method is verified also in the task of computing exit pathways for small molecules (ligand) from a protein.
Accession Number: WOS:000449334500089
Conference Title: 23rd IEEE International Conference on Emerging Technologies and Factory Automation (ETFA)
Conference Date: SEP 04-07, 2018
Conference Location: Politecnico Torino, Torino, ITALY
Conference Sponsors: Inst Elect & Elect Engineers, Inst Elect & Elect Engineers Ind Elect Soc, Natl Res Council Italy, Inst Elect Comp & Telecommunicat Engn
Conference Host: Politecnico Torino
ISSN: 1946-0740
ISBN: 978-1-5386-7108-5

Record 192 of 214
Title: Development and implementation of VoIP honeypots with wide range of analysis
Author(s): Behan, L (Behan, Ladislav); Kapicak, L (Kapicak, Lukas); Jalowiczor, J (Jalowiczor, Jakub)
Edited by: Ternovskiy IV; Chin P
Source: CYBER SENSING 2018 **Book Series:** Proceedings of SPIE **Volume:** 10630 **Article Number:** 106300S **DOI:** 10.1117/12.2304602 **Published:** 2018
Abstract: The paper deals with the need to provide security of the VoIP (Voice over IP) architecture. It is not entirely trivial matter to ensure the security of the VoIP services and attacks on telecommunication solutions, built on VoIP technology, grow with an increasing number of active users. In many situations, it is necessary to detect and analyze these attacks, monitor their progress and then prepare an effective defense against them. The best way how to detect attacks on VoIP infrastructure is implementing VoIP Honeypots. We have developed our honeypot solution. The main motivation for the development of our own honeypot for VoIP service is a nonexistent actively developed project with a similar purpose, which is adapted to the new security threats and which is developed according to the needs of the telecommunications market. Honeypot for VoIP services is implemented purely in software and honeypot is able to deal with various types of attacks. The entire solution is based on a Linux platform and it is prepared in a virtual environment for the simplest deployment and clustering possible.
Accession Number: WOS:000449558300021
Conference Title: Conference on Cyber Sensing
Conference Date: APR 17-18, 2018
Conference Location: Orlando, FL
Conference Sponsors: SPIE
ISSN: 0277-786X
eISSN: 1996-756X
ISBN: 978-1-5106-1772-8

Record 193 of 214
Title: Constitutive Models for Design of Sustainable Concrete Structures
Author(s): Brozovsky, J (Brozovsky, J.); Cajka, R (Cajka, R.); Koktan, J (Koktan, J.)
Edited by: Bui QB; Cajka R; Tran MT; Trinh TA; Yasar AUH; Wets G; Woloszyn M
Source: 2ND INTERNATIONAL CONFERENCE ON SUSTAINABLE DEVELOPMENT IN CIVIL, URBAN AND TRANSPORTATION ENGINEERING (CUTE 2018) **Book Series:** IOP Conference Series-Earth and Environmental Science **Volume:** 143 **Article Number:** UNSP 012036 **DOI:** 10.1088/1755-1315/143/1/012036 **Published:** 2018
Abstract: The paper deals with numerical models of reinforced concrete which are expected to be useful to enhance design of sustainable reinforced concrete structures. That is, the models which can deliver higher precision of results than the linear elastic models but which are still feasible for engineering practice. Such models can be based on an elastic-plastic material. The paper discusses properties of such models. A material model based of the Chen criteria and the Ohtani hardening model for concrete was selected for further development. There is also given a comparison of behaviour of such model with behaviour of a more complex smeared crack model which is based on principles of fracture mechanics.
Accession Number: WOS:000447721000036
Conference Title: 2nd International Conference on Sustainable Development in Civil, Urban and Transportation Engineering (CUTE)

Conference Date: APR 17-19, 2018
Conference Location: Ton Duc Thang Univ, Ho Chi Minh, VIETNAM
Conference Sponsors: Univ Savoie Mont Blanc, Hasselt Univ, Tech Univ Ostrava, Wroclaw Univ Technol, Univ Trieste
Conference Host: Ton Duc Thang Univ
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Cajka, Radim		0000-0002-2346-062X
Brozovsky, Jiri		0000-0001-6866-8718
Koktan, Jiri		0000-0003-1116-8362

ISSN: 1755-1307

Record 194 of 214
Title: Data-driven Construction of Symbolic Process Models for Reinforcement Learning
Author(s): Derner, E (Derner, Erik); Kubalik, J (Kubalik, Jiri); Babuska, R (Babuska, Robert)
Book Group Author(s): IEEE
Source: 2018 IEEE INTERNATIONAL CONFERENCE ON ROBOTICS AND AUTOMATION (ICRA) **Book Series:** IEEE International Conference on Robotics and Automation ICRA **Pages:** 5105-5112 **Published:** 2018

Abstract: Reinforcement learning (RL) is a suitable approach for controlling systems with unknown or time-varying dynamics. RL in principle does not require a model of the system, but before it learns an acceptable policy, it needs many unsuccessful trials, which real robots usually cannot withstand. It is well known that RL can be sped up and made safer by using models learned online. In this paper, we propose to use symbolic regression to construct compact, parsimonious models described by analytic equations, which are suitable for realtime robot control. Single node genetic programming (SNGP) is employed as a tool to automatically search for equations fitting the available data. We demonstrate the approach on two benchmark examples: a simulated mobile robot and the pendulum swing-up problem; the latter both in simulations and real-time experiments. The results show that through this approach we can find accurate models even for small batches of training data. Based on the symbolic model found, RL can control the system well.

Accession Number: WOS:000446394503126
Conference Title: IEEE International Conference on Robotics and Automation (ICRA)
Conference Date: MAY 21-25, 2018
Conference Location: Brisbane, AUSTRALIA
Conference Sponsors: IEEE, CSIRO, Australian Govt, Dept Def Sci & Technol, DJI, Queensland Univ Technol, Woodside, Baidu, Bosch, Houston Mechatron, Kinova Robot, KUKA, Hit Robot Grp, Honda Res Inst, iRobot, Mathworks, NuTonomy, Ouster, Uber
ISSN: 1050-4729
ISBN: 978-1-5386-3081-5

Record 195 of 214
Title: Theoretical Modelling of High-Resolution X-Ray Absorption Spectra at Uranium M-4 Edge
Author(s): Kolorenc, J (Kolorenc, Jindrich); Kvashnina, KO (Kvashnina, Kristina O.)
Source: MRS ADVANCES **Volume:** 3 **Issue:** 53 **Pages:** 3143-3148 **DOI:** 10.1557/adv.2018.470 **Published:** 2018

Abstract: We investigate the origin of satellite features that appear in the high-resolution x-ray absorption spectra measured at the uranium M-4 edge in compounds where the uranium atoms are in the U6+ oxidation state. We employ a material-specific Anderson impurity model derived from the electronic structure obtained by the density-functional theory.

Accession Number: WOS:000446896200001
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Kolorenc, Jindrich	G-5405-2014	0000-0003-2627-8302

ISSN: 2059-8521

Record 196 of 214
Title: Analysis of Mixed Workloads from Shared Cloud Infrastructure
Author(s): Klusacek, D (Klusacek, Dalibor); Parak, B (Parak, Boris)
Edited by: Klusacek D; Cirne W; Desai N
Source: JOB SCHEDULING STRATEGIES FOR PARALLEL PROCESSING, JSSPP 2017 **Book Series:** Lecture Notes in Computer Science **Volume:** 10773 **Pages:** 25-42 **DOI:** 10.1007/978-3-319-77398-8_2 **Published:** 2018

Abstract: Modern computing environments such as clouds, grids or HPC clusters are both complex and costly installations. Therefore, it has always been a major challenge to utilize them properly. Workload scheduling is a critical process in every production system with an unwanted potential to hamper overall performance if the given scheduler is not adequate or properly configured. Therefore, researchers as well as system administrators are frequently using historic workload traces to model/analyze the behavior of real systems in order to improve existing scheduling approaches. In this work we provide such real-life workload traces from the CERIT-SC system. Importantly, our traces describe a "mixed" workload consisting of both cloud VMs and grid jobs executed over a shared computing infrastructure. Provided workloads represent an interesting scheduling problem. First, these mixed workloads involving both "grid jobs" and cloud VMs increase the complexity of required (co)scheduling necessary to efficiently use the underlying physical infrastructure. Second, we also provide a detailed description of the setup of the system, its operational constraints and unresolved issues, putting the observed workloads into a broader context. Last but not least, the workloads are made freely available to the scientific community allowing for further independent research and analysis.

Accession Number: WOS:000444863700002
Conference Title: 21st International Workshop on Job Scheduling Strategies for Parallel Processing (JSSPP)
Conference Date: JUN 02, 2017
Conference Location: Orlando, FL
ISSN: 0302-9743
eISSN: 1611-3349
ISBN: 978-3-319-77398-8; 978-3-319-77397-1

Record 197 of 214
Title: Rayleigh Scattering as an Opacity Source in Stellar Atmospheres
Author(s): Fisak, J (Fisak, Jakub); Kubat, J (Kubat, Jiri); Krticka, J (Krticka, Jiri)
Edited by: Mendoza C; TurckChieze S; Colgan J
Source: WORKSHOP ON ASTROPHYSICAL OPACITIES **Book Series:** Astronomical Society of the Pacific Conference Series **Volume:** 515 **Pages:** 207-212 **Published:** 2018

Abstract: There are many different opacity sources in stellar atmospheres. Due to limited computational capabilities, the less important opacity sources are usually overlooked in stellar atmosphere models. Rayleigh scattering is frequently neglected in model atmospheres, which is not always valid. We study the influence of Rayleigh scattering by hydrogen and helium on computed stellar atmospheres of hot stars with solar chemical composition and of some types of chemically peculiar stars.

Accession Number: WOS:000442055300025
Conference Title: Workshop on Astrophysical Opacities
Conference Date: AUG 01-04, 2017
Conference Location: Western Michigan Univ, Foster Ctr, Kalamazoo, MI
Conference Sponsors: Western Michigan Univ, Coll Arts & Sci, Western Michigan Univ, Dept Phys
Conference Host: Western Michigan Univ, Foster Ctr
Author Identifiers:

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

ISSN: 1050-3390

ISBN: 978-1-58381-914-2

Record 198 of 214
Title: Lifted Relational Neural Networks: Efficient Learning of Latent Relational Structures
Author(s): Sourek, G (Sourek, Gustav); Aschenbrenner, V (Aschenbrenner, Vojtech); Zelezny, F (Zelezny, Filip); Schockaert, S (Schockaert, Steven); Kuzelka, O (Kuzelka, Ondrej)
Source: JOURNAL OF ARTIFICIAL INTELLIGENCE RESEARCH **Volume:** 62 **Pages:** 69-100 **Published:** 2018
Abstract: We propose a method to combine the interpretability and expressive power of first-order logic with the effectiveness of neural network learning. In particular, we introduce a lifted framework in which first-order rules are used to describe the structure of a given problem setting. These rules are then used as a template for constructing a number of neural networks, one for each training and testing example. As the different networks corresponding to different examples share their weights, these weights can be efficiently learned using stochastic gradient descent. Our framework provides a flexible way for implementing and combining a wide variety of modelling constructs. In particular, the use of first-order logic allows for a declarative specification of latent relational structures, which can then be efficiently discovered in a given data set using neural network learning. Experiments on 78 relational learning benchmarks clearly demonstrate the effectiveness of the framework.
Accession Number: WOS:000441027500003
ISSN: 1076-9757
eISSN: 1943-5037

Record 199 of 214
Title: Video Streaming to Empowered Video Walls
Author(s): Ubik, S (Ubik, Sven); Melnikov, J (Melnikov, Jiri); Travnicek, Z (Travnicek, Zdenek)
Source: INTERNATIONAL JOURNAL OF ELECTRONICS AND TELECOMMUNICATIONS **Volume:** 64 **Issue:** 3 **Pages:** 329-334 **DOI:** 10.24425/123526 **Published:** 2018
Abstract: Video walls are useful to display large size video content. Empowered video walls combine display functionality with computing power. Such video walls can display large scientific visualizations. If they can also display high-resolution video streamed over a network, they could enable distance collaboration over scientific data.
We proposed several methods of network streaming of high-resolution video content to a major type of empowered video walls, which is the SAGE2 system. For all methods, we evaluated their performance and discussed their scalability and properties. The results should be applicable to other web-based empowered video walls as well.
Accession Number: WOS:000440848700009
ISSN: 2081-8491
eISSN: 2300-1933

Record 200 of 214
Title: Towards Artificial Priority Queues for Similarity Query Execution
Author(s): Antol, M (Antol, Matej); Dohnal, V (Dohnal, Vlastislav)
Book Group Author(s): IEEE
Source: 2018 IEEE 34TH INTERNATIONAL CONFERENCE ON DATA ENGINEERING WORKSHOPS (ICDEW) **Pages:** 78-83 **DOI:** 10.1109/ICDEW.2018.00020 **Published:** 2018
Abstract: Content-based retrieval in large collections of unstructured data is challenging not only from the difficulty of the defining similarity between data images where the phenomenon of semantic gap appears, but also the efficiency of execution of similarity queries. Search engines providing similarity search typically organize various multimedia data, e.g. images of a photo stock, and support k-nearest neighbor query. Users accessing such systems then look for data items similar to their specific query object and refine results by re-running the search with an object from the previous query results. This paper is motivated by unsatisfactory query execution performance of indexing structures that use metric space as a convenient data model. We present performance behavior of two state-of-the-art representatives and propose a new universal technique for ordering priority queue of data partitions to be accessed during kNN query evaluation. We verify it in experiments on real-life data-sets.
Accession Number: WOS:000440300600014
Conference Title: 34th IEEE International Conference on Data Engineering Workshops (ICDEW)
Conference Date: APR 16-19, 2018
Conference Location: Paris, FRANCE
Conference Sponsors: IEEE, IEEE Comp Soc, U S Natl Sci Fdn
ISBN: 978-1-5386-6306-6

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Record 201 of 214

Title: Seeking the true Oscillatoria: a quest for a reliable phylogenetic and taxonomic reference point

Author(s): Muhlsteinova, R (Muhlsteinova, Radka); Hauer, T (Hauer, Tomas); De Ley, P (De Ley, Paul); Pietrasiak, N (Pietrasiak, Nicole)

Source: PRESLIA **Volume:** 90 **Issue:** 2 **Pages:** 151-169 **DOI:** 10.23855/preslia.2018.151 **Published:** 2018

Abstract: Reliable taxonomy of any group of organisms cannot be performed without phylogenetic reference points. In the historical "morphological era", a designated type specimen was considered fully sufficient but nowadays this principle can prove to be problematic and challenging especially when studying microscopic organisms. However, within the last decades there has been tremendous advancement in microscopy imaging and molecular biology offering additional data to systematic studies in ways that are revolutionizing cyanobacterial taxonomy. Unfortunately, most of the existing herbarium specimens or even iconotypes of old established taxa often cannot be subjects of modern analytic methods. Such is the case for the widely known cyanobacterial genus Oscillatoria which was introduced by Vaucher in 1803. In this study, we establish an epitype of the type species Oscillatoria princeps and provide an emended generic description based on data obtained from light as well as electron microscopy. We also present phylogenetic relationships of the genus Oscillatoria sensu stricto, a well-supported monophyletic Glade, to other related cyanobacterial taxa using DNA sequence data of the 16S rRNA gene region. Our epitypification of Oscillatoria and the establishment of a phylogenetic DNA benchmark will aid in improving the understanding of cyanobacterial diversity and deeper level taxonomy.

Accession Number: WOS:000439008500004

ISSN: 0032-7786

Record 202 of 214

Title: Studying coherent scattering in the CP stars atmospheres

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

Source: CONTRIBUTIONS OF THE ASTRONOMICAL OBSERVATORY SKALNATE PLESO **Volume:** 48 **Issue:** 1 **Pages:** 213-217 **Published:** 2018

Abstract: Chemically peculiar stars form a very interesting class of stars which frequently show variability. The variability is probably caused by the uneven surface distribution of chemical elements. Some elements are overabundant and some elements are underabundant compared to the solar chemical composition. In the case of chemically overabundant composition some of the rare photon atom processes can be more important than in the atmospheres of stars with solar chemical composition. We study the importance of Rayleigh scattering by helium.

Accession Number: WOS:000432791300030

Author Identifiers:

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ISSN: 1335-1842

eISSN: 1336-0337

Record 203 of 214

Title: Odd nuclei spectroscopy within a self-consistent multiphonon approach

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

Edited by: Gargano A; Coraggio L; Itaco N

Source: 12TH INTERNATIONAL SPRING SEMINAR ON NUCLEAR PHYSICS: CURRENT PROBLEMS AND PROSPECTS FOR NUCLEAR STRUCTURE **Book Series:** Journal of Physics Conference Series **Volume:** 966 **Article Number:** UNSP 012007 **DOI:** 10.1088/1742-6596/966/1/012007 **Published:** 2018

Abstract: The extension to odd nuclei of the equation of motion phonon method (EMPM) is briefly outlined. It derives and solves iteratively a set of equations of motion which yield an orthonormal basis of states composed of an odd particle coupled to orthonormal multiphonon states, also generated within the EMPM, describing the excitations of a doubly magic core. The basis so obtained is used to solve the eigenvalue problem in the full particle-phonon space. We have applied the method to the odd neighbors of O-16 using an optimized chiral potential in a space spanned by particle-core basis states which include up to three-phonons. The calculations have shown that the multiphonon states enhance enormously the density of levels and compress the whole spectrum, consistently with the data. They also contribute substantially to improve the agreement with the experimental moments and transitions strengths.

Accession Number: WOS:000431671600007

Conference Title: 12th International Spring Seminar on Nuclear Physics - Current Problems and Prospects for Nuclear Structure

Conference Date: MAY 15-19, 2017

Conference Location: ITALY

Conference Sponsors: Univ Napoli Federico II, Dipartimento Fisica Ettore Pancini, Ist Nazl Fisica Nucleare, Univ Napoli Federico II, Univ Campania Luigi Vanvitelli

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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ISSN: 1742-6588

Record 204 of 214

Title: Quasiparticle formulation of a multiphonon method and its application to the O-20 nucleus

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

Edited by: Gargano A; Coraggio L; Itaco N

Source: 12TH INTERNATIONAL SPRING SEMINAR ON NUCLEAR PHYSICS: CURRENT PROBLEMS AND PROSPECTS FOR NUCLEAR STRUCTURE **Book Series:** Journal of Physics Conference Series **Volume:** 966 **Article Number:** UNSP 012047 **DOI:** 10.1088/1742-6596/966/1/012047 **Published:** 2018

Abstract: We outline briefly the quasiparticle formulation of a microscopic multiphonon approach known as equation of motion phonon method and discuss its application to the neutron rich semi-magic O-20. Our calculation emphasizes the crucial role of the two-phonon configurations, responsible for establishing an almost one to one correspondence between theoretical and experimental energy levels and for fragmenting the dipole strength, in qualitative agreement with the data. In particular, the fragmentation yields two dipole levels below the neutron threshold which correspond to the two peaks recently observed.

Accession Number: WOS:000431671600047

Conference Title: 12th International Spring Seminar on Nuclear Physics - Current Problems and Prospects for Nuclear Structure

Conference Date: MAY 15-19, 2017

Conference Location: ITALY

Conference Sponsors: Univ Napoli Federico II, Dipartimento Fisica Ettore Pancini, Ist Nazl Fisica Nucleare, Univ Napoli Federico II, Univ Campania Luigi Vanvitelli

Author Identifiers:

Author	ResearcherID Number	ORCID Number
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ISSN: 1742-6588

Record 205 of 214

Title: Ab initio NMR parameters of BrCH3 and ICH3 with relativistic and vibrational corrections

Author(s): Uhlikova, T (Uhlikova, Tereza); Urban, S (Urban, Stepan)

Source: MOLECULAR PHYSICS **Volume:** 116 **Issue:** 9 **Pages:** 1192-1197 **DOI:** 10.1080/00268976.2017.1416194 **Published:** 2018

Abstract: This study is focused on two effects identified when NMR parameters are calculated based on first principles. These effects are 1. vibrational correction of properties when using ab initio optimized equilibrium geometry; 2. relativistic effects and limits of using the Flygare equation. These effects have been investigated and determined for nuclear spin-rotation constants and nuclear magnetic shieldings for the CH3Br and CH3I molecules. The most significant result is the difference between chemical shieldings determined based on the ab initio relativistic four-component Dirac-Coulomb Hamiltonian and chemical shieldings calculated using experimental values and the Flygare equation. This difference is approximately 320 ppm and 1290 ppm for Br-79 and I-127 in the CH3X molecule, respectively.

Accession Number: WOS:000430424300010
ISSN: 0026-8976
eISSN: 1362-3028

Record 206 of 214
Title: A detailed atomistic molecular simulation study on adsorption-based separation of CO2 using a porous coordination polymer
Author(s): Zarabadi-Poor, P (Zarabadi-Poor, Pezhman); Rocha-Rinza, T (Rocha-Rinza, Tomas)
Source: RSC ADVANCES **Volume:** 8 **Issue:** 26 **Pages:** 14144-14151 **DOI:** 10.1039/c8ra01408f **Published:** 2018

Abstract: Emission of CO2 is considered as one of the sources of global warming. Besides its currently inevitable production via several processes such as fuel consumption, it also exists in some other gaseous mixtures like biogas. Separation of carbon dioxide using solid adsorbents, for example porous coordination polymers and metal-organic frameworks, is an interesting active area of separation science. In particular, we performed detailed molecular simulations to investigate the response of a recently reported cobalt-based, pillared-layer, porous polymer on the CO2 separation from biogas, natural gas, and flue gas. The effect of the coordinated water molecules to the open metal sites on the corresponding properties was studied and revealed enhanced results even in comparison with HKUST-1. Additionally, our results provide insights on the role of -NO2 groups on the applications examined herein. Overall this study offers valuable insights about secondary building units of the examined materials which we expect to prove useful in the enhancement of carbon dioxide separation and capture.
Accession Number: WOS:000430536600002
Author Identifiers:

Author	ResearcherID Number	ORCID Number
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ISSN: 2046-2069

Record 207 of 214
Title: Magnetic field and forces in a pair of parallel conductors
Author(s): Coufal, O (Coufal, Oldrich); Radil, L (Radil, Lukas); Toman, P (Toman, Petr)
Source: INTERNATIONAL JOURNAL OF APPLIED ELECTROMAGNETICS AND MECHANICS **Volume:** 56 **Issue:** 2 **Pages:** 243-261 **DOI:** 10.3233/JAE-170077 **Published:** 2018

Abstract: The article provides a comprehensive idea of the calculating the magnetic field and forces in a pair of parallel solid conductors. The conductors are connected to a sinusoidal voltage source of a frequency that does not exceed 1 MHz. Thus the current density over the conductor cross sections is not constant. Its distribution depends on the distance of the conductors and their resistivity, on the shape of conductor cross sections, and on the voltage source frequency. The distribution of current density over the conductor cross sections affects not only the magnetic field produced by the conductors but also the forces acting on the conductors. For the acting forces, general conclusions are derived that hold for conductors of arbitrary shape of cross section. Specifically, pairs of conductors of rectangular, circular and triangular cross section are examined.
Accession Number: WOS:000426756400007
Author Identifiers:

Author	ResearcherID Number	ORCID Number
Toman, Petr	O-2269-2014	0000-0002-1708-009X

ISSN: 1383-5416
eISSN: 1875-8800

Record 208 of 214
Title: Simultaneous transmission of accurate time, stable frequency, data, and sensor system over one fiber with ITU 100 GHz grid
Author(s): Horvath, T (Horvath, Tomas); Munster, P (Munster, Petr); Vojtech, J (Vojtech, Josef); Velc, R (Velc, Radek); Oujezsky, V (Oujezsky, Vaclav)
Source: OPTICAL FIBER TECHNOLOGY **Volume:** 40 **Pages:** 139-143 **DOI:** 10.1016/j.yofte.2017.11.016 **Published:** JAN 2018

Abstract: Optical fiber is the most used medium for current telecommunication networks. Besides data transmissions, special advanced applications like accurate time or stable frequency transmissions are more common, especially in research and education networks. On the other hand, new applications like distributed sensing are in ISP's interest because e.g. such sensing allows new service: protection of fiber infrastructure. Transmission of all applications in a single fiber can be very cost efficient but it is necessary to evaluate possible interaction before real application and deploying the service, especially if standard 100 GHz grid is considered. We performed laboratory measurement of simultaneous transmission of 100 G data based on DP-QPSK modulation format, accurate time, stable frequency and sensing system based on phase sensitive OTDR through two types of optical fibers, G. 655 and G. 653. These fibers are less common than G. 652 fiber but thanks to their slightly higher nonlinear character, there are suitable for simulation of the worst case which can arise in a real network.
Accession Number: WOS:000425178200020
ISSN: 1068-5200
eISSN: 1095-9912

Record 209 of 214
Title: Rational Design of a New Class of Toll-Like Receptor 4 (TLR4) Tryptamine Related Agonists by Means of the Structure- and Ligand-Based Virtual Screening for Vaccine Adjuvant Discovery
Author(s): Honegr, J (Honegr, Jan); Dolezal, R (Dolezal, Rafael); Malinak, D (Malinak, David); Benkova, M (Benkova, Marketa); Soukup, O (Soukup, Ondrej); de Almeida, JSFD (de Almeida, Joyce S. F. D.); Franca, TCC (Franca, Tanos C. C.); Kuca, K (Kuca, Kamil); Prymula, R (Prymula, Roman)
Source: MOLECULES **Volume:** 23 **Issue:** 1 **Article Number:** 102 **DOI:** 10.3390/molecules23010102 **Published:** JAN 2018

Abstract: In order to identify novel lead structures for human toll-like receptor 4 (hTLR4) modulation virtual high throughput screening by a peta-flops-scale supercomputer has been performed. Based on the in silico studies, a series of 12 compounds related to tryptamine was rationally designed to retain suitable molecular geometry for interaction with the hTLR4 binding site as well as to satisfy general principles of drug-likeness. The proposed compounds were synthesized, and tested by in vitro and ex vivo experiments, which revealed that several of them are capable to stimulate hTLR4 in vitro up to 25% activity of Monophosphoryl lipid A. The specific affinity of the in vitro most potent substance was confirmed by surface plasmon resonance direct-binding experiments. Moreover, two compounds from the series show also significant ability to elicit production of interleukin 6.
Accession Number: WOS:000425082500097
PubMed ID: 29300367
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ISSN: 1420-3049

Record 210 of 214
Title: Stable Scalp EEG Spatiospectral Patterns Across Paradigms Estimated by Group ICA
Author(s): Labounek, R (Labounek, Rene); Bridwell, DA (Bridwell, David A.); Marecek, R (Marecek, Radek); Lamos, M (Lamos, Martin); Mikl, M (Mikl, Michal); Slavicek, T (Slavicek, Tomas); Bednarik, P (Bednarik, Petr); Bastinec, J (Bastinec, Jaromir); Hlustik, P (Hlustik, Petr); Brazdil, M (Brazdil, Milan); Jan, J (Jan, Jiri)
Source: BRAIN TOPOGRAPHY **Volume:** 31 **Issue:** 1 **Special Issue:** SI **Pages:** 76-89 **DOI:** 10.1007/s10548-017-0585-8 **Published:** JAN 2018

Abstract: Electroencephalography (EEG) oscillations reflect the superposition of different cortical sources with potentially different frequencies. Various blind source separation (BSS) approaches have been developed and implemented in order to decompose these oscillations, and a subset of approaches have been developed for decomposition of multi-subject data. Group independent component analysis (Group ICA) is one such approach, revealing spatiospectral maps at the group level with distinct frequency and spatial characteristics. The reproducibility of these distinct maps across subjects and paradigms is relatively unexplored domain, and the topic of the present study. To address this, we conducted separate group ICA decompositions of EEG spatiospectral patterns on data collected during three different paradigms or tasks (resting-state, semantic decision task and visual oddball task). K-means clustering analysis of back-reconstructed individual subject maps demonstrates that fourteen different independent spatiospectral maps are present across the different paradigms/tasks, i.e. they are generally stable.

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Labounek, Rene		0000-0003-0439-1304

Record 211 of 214

Title: Behavior of BsoBI endonuclease in the presence and absence of DNA

Author(s): Stepan, J (Stepan, Jakub); Kabelka, I (Kabelka, Ivo); Koca, J (Koca, Jaroslav); Kulhanek, P (Kulhanek, Petr)

Source: JOURNAL OF MOLECULAR MODELING **Volume:** 24 **Issue:** 1 **Article Number:** 22 **DOI:** 10.1007/s00894-017-3557-8 **Published:** JAN 2018

Abstract: BsoBI is a type II restriction endonuclease belonging to the EcoRI family. There is only one previously published X-ray structure for this endonuclease: it shows a homodimer of BsoBI completely encircling DNA in a tunnel. In this work, molecular dynamics simulations were employed to elucidate possible ways in which DNA is loaded into this complex prior to its cleavage. We found that the dimer does not open spontaneously when DNA is removed from the complex on the timescale of our simulations (similar to 0.5 mu s). A biased simulation had to be used to facilitate the opening, which revealed a possible way for the two catalytic domains to separate. The alpha-helices connecting the catalytic and helical domains were found to act as a hinge during the separation. In addition, we found that the opening of the BsoBI dimer was influenced by the type of counterions present in the environment. A reference simulation of the BsoBI/DNA complex further showed spontaneous reorganization of the active sites due to the binding of solvent ions, which led to an active-site structure consistent with other experimental structures of type II restriction endonucleases determined in the presence of metal ions.

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Author	ResearcherID Number	ORCID Number
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Kulhanek, Petr	D-6884-2012	0000-0002-4152-6514

Record 212 of 214

Title: Glacial refugia and postglacial spread of an iconic large European land snail, Helix pomatia (Pulmonata: Helicidae)

Author(s): Korabek, O (Korabek, Ondrej); Petrusek, A (Petrusek, Adam); Jurickova, L (Jurickova, Lucie)

Source: BIOLOGICAL JOURNAL OF THE LINNEAN SOCIETY **Volume:** 123 **Issue:** 1 **Pages:** 218-234 **DOI:** 10.1093/biolinnean/blx135 **Published:** JAN 2018

Abstract: The Holocene postglacial expansions offer a possibility to assess how quickly snails, with proverbially slow active dispersal and unclear passive dispersal capabilities, can naturally spread. We explore the possibilities and limitations of such an approach on an iconic European snail. We locate probable sources of postglacial expansion of Helix pomatia and date its earliest postglacial subfossil occurrences in Central Europe, close to presumed natural northern distribution limits. With dense sampling of the species native range, we found most of its mitochondrial diversity at c. 45 degrees N or more southerly. A hotspot in Bosnia and Serbia contributed to colonization of the Pannonian Basin, Carpathians and Bohemian Massif; however, the most widely distributed lineage has a more westerly centre of diversity, with a possible refugium in Italy. We revised the oldest occurrences post-dating the Late Pleniglacial from Czechia and Slovakia suggested by literature and radiocarbon-dated the preserved shell fragments. No reliably identified fragment yielded a date earlier than 10 121-9695 cal BP. Stratigraphy-based records presumed older turned out to be unreliable, making the argument for a direct dating approach. However, our results confirm that in the absence of northern refugia, H. pomatia must have been able to colonize the newly emerging postglacial habitats rapidly.

Author Identifiers:

Author	ResearcherID Number	ORCID Number
Petrusek, Adam	A-3510-2008	0000-0001-5150-4370
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Record 213 of 214

Title: Staphylococcus edaphicus sp nov., Isolated in Antarctica, Harbors the mecC Gene and Genomic Islands with a Suspected Role in Adaptation to Extreme Environments

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Source: APPLIED AND ENVIRONMENTAL MICROBIOLOGY **Volume:** 84 **Issue:** 2 **Article Number:** UNSP e01746-17 **DOI:** 10.1128/AEM.01746-17 **Published:** JAN 2018

Abstract: Two Gram-stain-positive, coagulase-negative staphylococcal strains were isolated from abiotic sources comprising stone fragments and sandy soil in James Ross Island, Antarctica. Here, we describe properties of a novel species of the genus Staphylococcus that has a 16S rRNA gene sequence nearly identical to that of Staphylococcus saprophyticus. However, compared to S. saprophyticus and the next closest relatives, the new species demonstrates considerable phylogenetic distance at the whole-genome level, with an average nucleotide identity of <85% and inferred DNA-DNA hybridization of <30%. It forms a separate branch in the S. saprophyticus phylogenetic clade as confirmed by multilocus sequence analysis of six housekeeping genes, rpoB, hsp60, tuf, dnaJ, gap, and sod. Matrix-assisted laser desorption ionization-time of flight mass spectrometry (MALDI-TOF MS) and key biochemical characteristics allowed these bacteria to be distinguished from their nearest phylogenetic neighbors. In contrast to S. saprophyticus subsp. saprophyticus, the novel strains are pyrrolidonyl arylamidase and beta-glucuronidase positive and beta-galactosidase negative, nitrate is reduced, and acid produced aerobically from D-mannose. Whole-genome sequencing of the 2.69-Mb large chromosome revealed the presence of a number of mobile genetic elements, including the 27-kb pseudo-staphylococcus cassette chromosome mec of strain P5085(T) (psi SCCmec(P5085)), harboring the mecC gene, two composite phage-inducible chromosomal islands probably essential to adaptation to extreme environments, and one complete and one defective prophage. Both strains are resistant to penicillin G, ampicillin, ceftazidime, methicillin, cefoxitin, and fosfomycin. We hypothesize that antibiotic resistance might represent an evolutionary advantage against beta-lactam producers, which are common in a polar environment. Based on these results, a novel species of the genus Staphylococcus is described and named Staphylococcus edaphicus sp. nov. The type strain is P5085(T) (= CCM 8730(T) = DSM 104441(T)).
IMPORTANCE The description of Staphylococcus edaphicus sp. nov. enables the comparison of multidrug-resistant staphylococci from human and veterinary sources evolved in the globalized world to their geographically distant relative from the extreme Antarctic environment. Although this new species was not exposed to the pressure of antibiotic treatment in human or veterinary practice, mobile genetic elements carrying antimicrobial resistance genes were found in the genome. The genomic characteristics presented here elucidate the evolutionary relationships in the Staphylococcus genus with a special focus on antimicrobial resistance, pathogenicity, and survival traits. Genes encoded on mobile genetic elements were arranged in unique combinations but retained conserved locations for the integration of mobile genetic elements. These findings point to enormous plasticity of the staphylococcal pangenome, shaped by horizontal gene transfer. Thus, S. edaphicus can act not only as a reservoir of antibiotic resistance in a natural environment but also as a mediator for the spread and evolution of resistance genes.

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Title: Ecological controls of mammalian diversification vary with phylogenetic scale

Author(s): Machac, A (Machac, Antonin); Graham, CH (Graham, Catherine H.); Storch, D (Storch, David)

Source: GLOBAL ECOLOGY AND BIOGEOGRAPHY **Volume:** 27 **Issue:** 1 **Pages:** 32-46 **DOI:** 10.1111/geb.12642 **Published:** JAN 2018

Abstract: Aim: Diversity dynamics remain controversial. Here, we examine these dynamics, together with the ecological factors governing them, across mammalian clades of different ages and sizes, representing different phylogenetic scales. Specifically, we investigate whether the dynamics are bounded or unbounded, biotically or abiotically regulated, stochastic or ecologically deterministic.

Location: Worldwide.

Time period: 150 Myr.

Major taxa studied: Mammals.

Methods: Integrating the newest phylogenetic and distributional data by means of several distinct methods, we study the ecology of mammalian diversification within a predictive framework, inspired by classic theory. Specifically, we evaluate the effects of several classes of factors, including climate, topography, geographical area, rates of climatic-niche evolution, and regional coexistence between related and unrelated species. Next, we determine whether the relative effects of these factors change systematically across clades representing different phylogenetic scales.

Results: We find that young clades diversify at approximately constant rates, medium-sized clades show diversification slowdowns, and large clades are mostly saturated, suggesting that diversification dynamics change as clades grow and accumulate species. We further find that diversification slowdowns intensify with the degree of regional coexistence between related species, presumably because increased competition for regional resources suppresses the diversification process. The richness at which clades eventually saturate depends on climate; clades residing in tropical climates saturate at low richness, implying that niches become progressively densely packed towards the tropics.

Main conclusions: The diversification process is influenced by a variety of ecological factors, whose relative effects change across phylogenetic scales, producing scale-dependent dynamics. Different segments of the same phylogeny might therefore support seemingly conflicting results (bounded or unbounded, biotically or abiotically regulated, stochastic or ecologically deterministic diversification), which might have contributed to several outstanding controversies in the field. These conflicts can be reconciled, however, when accounting for phylogenetic scale, which might, in turn, produce a more integrated understanding of global diversity dynamics.

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