

## Record 1 of 236

**Title:** Tailoring topological order and pi-conjugation to engineer quasi-metallic polymers**Author(s):** Cirera, B (Cirera, Borja); Sanchez-Grande, A (Sanchez-Grande, Ana); de la Torre, B (de la Torre, Bruno); Santos, J (Santos, Jose); Edalatmanesh, S (Edalatmanesh, Shayan); Rodriguez-Sanchez, E (Rodriguez-Sanchez, Eider); Lauwaet, K (Lauwaet, Koen); Mallada, B (Mallada, Benjamin); Zboril, R (Zboril, Radek); Miranda, R (Miranda, Rodolfo); Groning, O (Groning, Oliver); Jelinek, P (Jelinek, Pavel); Martin, N (Martin, Nazario); Ecija, D (Ecija, David)**Source:** NATURE NANOTECHNOLOGY Volume: 15 Issue: 6 Pages: 437-+ DOI: 10.1038/s41565-020-0668-7 Early Access Date: APR 2020 Published: JUN 2020**Abstract:** Topological band theory predicts that a topological electronic phase transition between two insulators must proceed via closure of the electronic gap. Here, we use this transition to circumvent the instability of metallic phases in pi-conjugated one-dimensional (1D) polymers. By means of density functional theory, tight-binding and GW calculations, we predict polymers near the topological transition from a trivial to a non-trivial quantum phase. We then use on-surface synthesis with custom-designed precursors to make polymers consisting of 1D linearly bridged acene moieties, which feature narrow bandgaps and in-gap zero-energy edge states when in the topologically non-trivial phase close to the topological transition point. We also reveal the fundamental connection between topological classes and resonant forms of 1D pi-conjugated polymers. Polymers commonly are semiconducting or insulating because of a sizable energy gap in the density of states around the Fermi level. Yet, the phase transition from topologically trivial to non-trivial in on-surface synthesized pi-conjugated polymers, due to a change of resonant form, stabilizes narrow bandgaps and bears in-gap zero-energy edge states in the non-trivial phase.**Accession Number:** WOS:000528019500003**PubMed ID:** 32313219**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Santos, Jose	K-1119-2014	0000-0002-9702-2315
Faes, Benjamin Mallada	T-6344-2019	0000-0002-8209-9977
De la Torre, Bruno	R-4536-2019	
Jelinek, Pavel	ABE-8589-2020	0000-0002-5645-8542
Grande, Ana Sanchez	ABH-3437-2020	
Zboril, Radek		0000-0002-3147-2196
Lauwaet, Koen	K-8624-2015	0000-0003-1024-6779
Edalatmanesh, Shayan		0000-0002-9095-1525
de la Torre, Bruno		0000-0002-6462-6833

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## Record 2 of 236

**Title:** Relativistic Heavy-Neighbor-Atom Effects on NMR Shifts: Concepts and Trends Across the Periodic Table**Author(s):** Vicha, J (Vicha, Jan); Novotny, J (Novotny, Jan); Komorovsky, S (Komorovsky, Stanislav); Straka, M (Straka, Michal); Kaupp, M (Kaupp, Martin); Marek, R (Marek, Radek)**Source:** CHEMICAL REVIEWS Volume: 120 Issue: 15 Pages: 7065-7103 DOI: 10.1021/acs.chemrev.9b00785 Published: AUG 12 2020**Abstract:** Chemical shifts present crucial information about an NMR spectrum. They show the influence of the chemical environment on the nuclei being probed. Relativistic effects caused by the presence of an atom of a heavy element in a compound can appreciably, even drastically, alter the NMR shifts of the nearby nuclei. A fundamental understanding of such relativistic effects on NMR shifts is important in many branches of chemical and physical science. This review provides a comprehensive overview, of the tools, concepts, and periodic trends pertaining to the shielding effects by a neighboring heavy atom in diamagnetic systems, with particular emphasis on the "spin-orbit heavy-atom effect on the light-atom" NMR shift (SO-HALA effect). The analyses and tools described in this review provide guidelines to help NMR spectroscopists and computational chemists estimate the ranges of the NMR shifts for an unknown compound, identify intermediates in catalytic and other processes, analyze conformational aspects and intermolecular interactions, and predict trends in series of compounds throughout the Periodic Table. The present review provides a current snapshot of this important subfield of NMR spectroscopy and a basis and framework for including future findings in the field.**Accession Number:** WOS:000562192900001**PubMed ID:** 32574047**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Novotny, Jan	D-7676-2012	0000-0002-1203-9549
Kaupp, Martin Prof. Dr.	K-9569-2016	0000-0003-1582-2819
Novotny, Jan	AAW-8723-2020	
Vicha, Jan	D-8417-2012	0000-0003-3698-8236
Straka, Michal	E-5246-2011	0000-0002-7857-4990
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Komorovsky, Stanislav	N-4332-2016	0000-0002-5317-7200

**ISSN:** 0009-2665**eISSN:** 1520-6890

## Record 3 of 236

**Title:** Giant radio galaxies in the LOFAR Two-metre Sky Survey I. Radio and environmental properties**Author(s):** Dabhade, P (Dabhade, P); Rottgering, HJA (Rottgering, H. J. A.); Bagchi, J (Bagchi, J.); Shimwell, TW (Shimwell, T. W.); Hardcastle, MJ (Hardcastle, M. J.); Sankhyayan, S (Sankhyayan, S.); Morganti, R (Morganti, R.); Jamrozy, M (Jamrozy, M.); Shulevski, A (Shulevski, A.); Duncan, KJ (Duncan, K. J.)**Source:** ASTRONOMY & ASTROPHYSICS Volume: 635 Article Number: A5 DOI: 10.1051/0004-6361/201935589 Published: FEB 28 2020**Abstract:** Giant radio galaxies (GRGs) are a subclass of radio galaxies, which have grown to megaparsec scales. GRGs are much rarer than normal-sized radio galaxies (< 0.7 Mpc) and the reason for their gigantic sizes is still debated. Here, we report on the biggest sample of GRGs identified to date. These objects were found in the LOFAR Two-metre Sky Survey first data release images, which cover a 424 deg(2) region. Of the 239 GRGs found, 225 are new discoveries. The GRGs in our sample have sizes ranging from 0.7 Mpc to 3.5 Mpc and have redshifts (z) between 0.1 and 2.3. Seven GRGs have sizes above 2 Mpc and one has a size of similar to 3.5 Mpc. The sample contains 40 GRGs hosted by spectroscopically confirmed quasars. Here, we present the search techniques employed and the resulting catalogue of the newly discovered large sample of GRGs along with their radio properties. In this paper, we also show for the first time that the spectral index of GRGs is similar to that of normal-sized radio galaxies, indicating that most of the GRG population is not dead or is not similar to a remnant-type radio galaxy. We find that 20 out of 239 GRGs in our sample are located at the centres of clusters and we present our analysis on their cluster environment and radio morphology.**Accession Number:** WOS:000518585100011**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Hardcastle, Martin	AAM-1395-2020	
Jamrozy, Marek	AAH-2495-2020	0000-0002-0870-7778
Hardcastle, Martin	E-2264-2012	0000-0003-4223-1117
Dabhade, Pratik		0000-0001-9212-3574
Shulevski, Aleksandar	E-5591-2015	0000-0002-1827-0469
Bagchi, Joydeep		0000-0002-2922-2884
Sankhyayan, Shishir		0000-0003-2601-2707
Morganti, Raffaella		0000-0002-9482-6844

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## Record 4 of 236

**Title:** Synthesis, in vitro screening and molecular docking of isoquinolinium-5-carbaldoximes as acetylcholinesterase and butyrylcholinesterase reactivators

**Author(s):** Malinak, D (Malinak, David); Dolezal, R (Dolezal, Rafael); Hepnarova, V (Hepnarova, Vendula); Hozova, M (Hozova, Miroslava); Andrys, R (Andrys, Rudolf); Bzonek, P (Bzonek, Petr); Racakova, V (Racakova, Veronika); Korabecny, J (Korabecny, Jan); Gorecki, L (Gorecki, Lukas); Mezeiova, E (Mezeiova, Eva); Psootka, M (Psootka, Miroslav); Jun, D (Jun, Daniel); Kuca, K (Kuca, Kamil); Musilek, K (Musilek, Kamil)

**Source:** JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY **Volume:** 35 **Issue:** 1 **Pages:** 478-488 **DOI:** 10.1080/14756366.2019.1710501 **Published:** JAN 1 2020

**Abstract:** The series of symmetrical and unsymmetrical isoquinolinium-5-carbaldoximes was designed and prepared for cholinesterase reactivation purposes. The novel compounds were evaluated for intrinsic acetylcholinesterase (AChE) or butyrylcholinesterase (BChE) inhibition, when the majority of novel compounds resulted with high inhibition of both enzymes and only weak inhibitors were selected for reactivation experiments on human AChE or BChE inhibited by sarin, VX, or paraoxon. The AChE reactivation for all used organophosphates was found negligible if compared to the reactivation ability of obidoxime. Importantly, two compounds were found to reactivate BChE inhibited by sarin or VX better to obidoxime at human attainable concentration. One compound resulted as better reactivator of NEMP (VX surrogate)-inhibited BChE than obidoxime. The in vitro results were further rationalized by molecular docking studies showing future directions on designing potent BChE reactivators.

**Accession Number:** WOS:000506063900001

**PubMed ID:** 31910701

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Malinak, David	AAH-1337-2020	
Dolezal, Rafael	B-3956-2017	0000-0001-9495-3934
Gorecki, Lukas	N-9017-2019	0000-0002-4791-6556
Sepsova, Vendula	L-7284-2017	0000-0002-6445-2669
Malinak, David		0000-0002-0665-0667
Korabecny, Jan	J-6362-2018	0000-0001-6977-7596
Reis, AlessanRSS		0000-0001-8486-7469
Musilek, Kamil	G-4258-2018	0000-0002-7504-4062

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#### Record 5 of 236

**Title:** CaverDock: A Novel Method for the Fast Analysis of Ligand Transport

**Author(s):** Filipovic, J (Filipovic, Jiri); Vavra, O (Vavra, Ondrej); Plhak, J (Plhak, Jan); Bednar, D (Bednar, David); Marques, SM (Marques, Sergio M.); Brezovsky, J (Brezovsky, Jan); Matyska, L (Matyska, Ludek); Damborsky, J (Damborsky, Jiri)

**Source:** IEEE-ACM TRANSACTIONS ON COMPUTATIONAL BIOLOGY AND BIOINFORMATICS **Volume:** 17 **Issue:** 5 **Pages:** 1625-1638 **DOI:** 10.1109/TCBB.2019.2907492 **Published:** SEPT 1 2020

**Abstract:** Here we present a novel method for the analysis of transport processes in proteins and its implementation called CaverDock. Our method is based on a modified molecular docking algorithm. It iteratively places the ligand along the access tunnel in such a way that the ligand movement is contiguous and the energy is minimized. The result of CaverDock calculation is a ligand trajectory and an energy profile of transport process. CaverDock uses the modified docking program Autodock Vina for molecular docking and implements a parallel heuristic algorithm for searching the space of possible trajectories. Our method lies in between the geometrical approaches and molecular dynamics simulations. Contrary to the geometrical methods, it provides an evaluation of chemical forces. However, it is far less computationally demanding and easier to set up compared to molecular dynamics simulations. CaverDock will find a broad use in the fields of computational enzymology, drug design, and protein engineering. The software is available free of charge to the academic users at <https://loschmidt.chemi.muni.cz/caverdock/>.

**Accession Number:** WOS:000576418300015

**PubMed ID:** 30932844

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Brezovsky, Jan	C-8290-2012	0000-0001-9677-5078
Bednar, David	ABF-5943-2020	0000-0002-6803-0340
Marques, Sergio M	H-8685-2012	0000-0002-6281-7505
Filipovic, Jiri	H-4311-2013	0000-0002-5703-9673

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#### Record 6 of 236

**Title:** Relativity or aromaticity? A first-principles perspective of chemical shifts in osmabenzene and osmapentalene derivatives

**Author(s):** Foroutan-Nejad, C (Foroutan-Nejad, Cina); Vicha, J (Vicha, Jan); Ghosh, A (Ghosh, Abhik)

**Source:** PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 22 **Issue:** 19 **Pages:** 10863-10869 **DOI:** 10.1039/d0cp01481h **Published:** MAY 21 2020

**Abstract:** We have studied the magnetic response properties and aromaticity of osmium metallacycles by means of scalar-relativistic (1c) and fully relativistic (4c) density functional theory computations. For osmabenzene, whose aromatic character is controversial, a topological analysis of the current density has revealed the presence of a unique sigma-type Craig-Mobius magnetic aromaticity. We show that the partially filled osmium valence shell induces a large paratropic current, which may interfere with certain methods commonly used to analyze aromaticity, in particular NICS. Further, we show that the extreme deshielding of the light atoms in the vicinity of the osmium atoms in osmapentalene derivatives is not a consequence of aromaticity but can be explained by paramagnetic couplings between sigma(Os-C) bonding orbitals and the pi\*(Os) orbitals. We demonstrate that variations in the orientation of the induced magnetic currents through the molecule dictates the alternating signs of the spin-orbit contribution to the NMR chemical shift.

**Accession Number:** WOS:000537251100044

**PubMed ID:** 32369060

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Vicha, Jan	D-8417-2012	0000-0003-3698-8236
Ghosh, Abhik	G-8164-2016	0000-0003-1161-6364
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173

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#### Record 7 of 236

**Title:** Simulation of Raman and Raman optical activity of saccharides in solution

**Author(s):** Palivec, V (Palivec, Vladimir); Kopecky, V (Kopecky, Vladimir, Jr.); Jungwirth, P (Jungwirth, Pavel); Bour, P (Bour, Petr); Kaminsky, J (Kaminsky, Jakub); Martinez-Seara, H (Martinez-Seara, Hector)

**Source:** PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 22 **Issue:** 4 **Pages:** 1983-1993 **DOI:** 10.1039/c9cp05682c **Published:** JAN 28 2020

**Abstract:** Structural studies of sugars in solution are challenging for most of the traditional analytical techniques. Raman and Raman optical activity (ROA) spectroscopies were found to be extremely convenient for this purpose. However, Raman and ROA spectra of saccharides are challenging to interpret and model due to saccharides' flexibility and polarity. In this study, we present an optimized computational protocol that enables the simulation of the spectra efficiently. Our protocol, which results in good agreement with experiments, combines molecular dynamics and density functional theory calculations. It further uses a smart optimization procedure and a novel adaptable scaling function. The numerical stability and accuracy of individual computational steps are evaluated by comparing simulated and experimental spectra of d-glucose, d-glucuronic acid, N-acetyl-d-glucosamine, methyl beta-d-glucopyranoside, methyl beta-d-glucuronide, and methyl beta-N-acetyl-d-glucosaminide. Overall, our Raman and ROA simulation protocol allows one to routinely and reliably calculate the spectra of small saccharides and opens the door to advanced applications, such as complete 3-dimensional structural determination by direct interpretation of the experimental spectra.

**Accession Number:** WOS:000510729400014

**PubMed ID:** 31930255

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kopecky, Vladimir	A-6965-2008	0000-0002-7331-9018
Jungwirth, Pavel	D-9290-2011	0000-0002-6892-3288
Kaminsky, Jakub	G-5672-2014	0000-0001-6347-3022
Palivec, Vladimir		0000-0003-0297-715X
Martinez-Seara, Hector	D-3734-2014	0000-0001-9716-1713

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**Record 8 of 236****Title:** Zeta Potential Determination from Molecular Simulations**Author(s):** Biriukov, D (Biriukov, Denys); Fibich, P (Fibich, Pavel); Predota, M (Predota, Milan)**Source:** JOURNAL OF PHYSICAL CHEMISTRY C Volume: 124 Issue: 5 Pages: 3159-3170 DOI: 10.1021/acs.jpcc.9b11371 Published: FEB 6 2020

**Abstract:** zeta-Potential (ZP) is among key physical properties characterizing the behavior of nanoparticles in colloidal solutions. Despite many attempts to calculate and neatly interpret the ZP, a full understanding of various factors influencing its values has not been achieved yet, even for standard metal oxides, particularly when considering high ionic concentrations and the effect of temperature. This contribution extends our recent work [Predota, M. et al. Langmuir 2016, 32, 10189-10198], where we suggested a direct approach to calculate the ZP from nonequilibrium molecular dynamics (NEMD) simulations. Here, we investigate NaCl, RbCl, CaCl<sub>2</sub>, SrCl<sub>2</sub>, and Na<sub>2</sub>C<sub>2</sub>O<sub>4</sub> aqueous solutions interacting with TiO<sub>2</sub> and SiO<sub>2</sub> surfaces and show contrasting ZP behaviors of these metal oxides, elucidated by theoretical insights gained by molecular simulations. We show that both surface-specific and ion-specific properties play a key role in the observed electrokinetics. Additionally, we explore the concentration and temperature influence on the ZP of selected systems and discuss the measurement of the ZP of systems with surfaces and ions modeled using scaled partial charges. Our results agree well with available experimental data and capture all key ZP features predicted by theory or revealed by experiments and advance the microscopic description of solid/liquid interfaces, promoting further applications of the suggested NEMD approach.

**Accession Number:** WOS:000512222000043**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Fibich, Pavel	B-3013-2015	0000-0001-9066-3753
Biriukov, Denys	Q-4898-2018	0000-0003-1007-2203
Predota, Milan	A-2256-2009	0000-0003-3902-0992

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**Record 9 of 236****Title:** Magainin 2 and PGLa in Bacterial Membrane Mimics II: Membrane Fusion and Sponge Phase Formation**Author(s):** Kabelka, I (Kabelka, Ivo); Pachler, M (Pachler, Michael); Prevost, S (Prevost, Sylvain); Letofsky-Papst, I (Letofsky-Papst, Ilse); Lohner, K (Lohner, Karl); Pabst, G (Pabst, Georg); Vacha, R (Vacha, Robert)**Source:** BIOPHYSICAL JOURNAL Volume: 118 Issue: 3 Pages: 612-623 DOI: 10.1016/j.bpj.2019.12.019 Published: FEB 4 2020

**Abstract:** We studied the synergistic mechanism of equimolar mixtures of magainin 2 (MG2a) and PGLa in phosphatidylethanolamine/phosphatidylglycerol mimics of Gram-negative cytoplasmic membranes. In a preceding article of this series, we reported on the early onset of parallel heterodimer formation of the two antimicrobial peptides already at low concentrations and the resulting defect formation in the membranes. Here, we focus on the structures of the peptide-lipid aggregates occurring in the synergistic regime at elevated peptide concentrations. Using a combination of calorimetric, scattering, electron microscopic, and in silico techniques, we demonstrate that the two peptides, even if applied individually, transform originally large unilamellar vesicles into multilamellar vesicles with a collapsed interbilayer spacing resulting from peptide-induced adhesion. Interestingly, the adhesion does not lead to a peptide-induced lipid separation of charged and charge-neutral species. In addition to this behavior, equimolar mixtures of MG2a and PGLa formed surface-aligned fibril-like structures, which induced adhesion zones between the membranes and the formation of transient fusion stalks in molecular dynamics simulations and a coexisting sponge phase observed by small-angle x-ray scattering. The previously reported increased leakage of lipid vesicles of identical composition in the presence of MG2a/PGLa mixtures is therefore related to a peptide-induced cross-linking of bilayers.

**Accession Number:** WOS:000511291400010**PubMed ID:** 31952806**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pabst, Georg	I-6919-2015	0000-0003-1967-1536

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**Record 10 of 236****Title:** DSS1 interacts with and stimulates RAD52 to promote the repair of DSBs**Author(s):** Stefanovie, B (Stefanovie, Barbora); Hengel, SR (Hengel, Sarah R.); Mlcouskova, J (Mlcouskova, Jarmila); Prochazkova, J (Prochazkova, Jana); Spirek, M (Spirek, Mario); Nikulenkov, F (Nikulenkov, Fedor); Nemecek, D (Nemecek, Daniel); Koch, BG (Koch, Brandon G.); Bain, FE (Bain, Fletcher E.); Yu, LP (Yu, Liping); Spies, M (Spies, Maria); Krejci, L (Krejci, Lumir)**Source:** NUCLEIC ACIDS RESEARCH Volume: 48 Issue: 2 Pages: 694-708 DOI: 10.1093/nar/gkz1052 Published: JAN 24 2020

**Abstract:** The proper repair of deleterious DNA lesions such as double strand breaks prevents genomic instability and carcinogenesis. In yeast, the Rad52 protein mediates DSB repair via homologous recombination. In mammalian cells, despite the presence of the RAD52 protein, the tumour suppressor protein BRCA2 acts as the predominant mediator during homologous recombination. For decades, it has been believed that the RAD52 protein played only a back-up role in the repair of DSBs performing an error-prone single strand annealing (SSA). Recent studies have identified several new functions of the RAD52 protein and have drawn attention to its important role in genome maintenance. Here, we show that RAD52 activities are enhanced by interacting with a small and highly acidic protein called DSS1. Binding of DSS1 to RAD52 changes the RAD52 oligomeric conformation, modulates its DNA binding properties, stimulates SSA activity and promotes strand invasion. Our work introduces for the first time RAD52 as another interacting partner of DSS1 and shows that both proteins are important players in the SSA and BIR pathways of DSB repair.

**Accession Number:** WOS:000518532100019**PubMed ID:** 31799622**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Krejci, Lumir	B-7842-2009	0000-0002-4732-1405

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**Record 11 of 236****Title:** Planet-Star Interactions with Precise Transit Timing. II. The Radial-Velocity Tides and a Tighter Constraint on the Orbital Decay Rate in the WASP-18 System**Author(s):** Maciejewski, G (Maciejewski, G.); Knutson, HA (Knutson, H. A.); Howard, AW (Howard, A. W.); Isaacson, H (Isaacson, H.); Fernandez-Lajus, E (Fernandez-Lajus, E.); Di Sisto, RP (Di Sisto, R. P.); Migaszewski, C (Migaszewski, C.)**Source:** ACTA ASTRONOMICA Volume: 70 Issue: 1 Pages: 1-18 DOI: 10.32023/0001-5237/70.1.1 Published: 2020

**Abstract:** From its discovery, the WASP-18 system with its massive transiting planet on a tight orbit was identified as a unique laboratory for studies on tidal planet-star interactions. In an analysis of Doppler data, which include five new measurements obtained with the HIRES/Keck-I instrument between 2012 and 2018, we show that the radial velocity signal of the photosphere following the planetary tidal potential can be distilled for the host star. Its amplitude is in agreement with both theoretical predictions of the equilibrium tide approximation and an ellipsoidal modulation observed in an orbital phase curve. Assuming a circular orbit, we refine system parameters using photometric time series from TESS. With a new ground-based photometric observation, we extend the span of transit timing observations to 28 yr in order to probe the rate of the orbital period shortening. Since we found no departure from a constant-period model, we conclude that the modified tidal quality parameter of the host star must be greater than  $3.9 \times 10^{10}$  with 95% confidence. This



result is in line with conclusions drawn from studies of the population of hot Jupiters, predicting that the efficiency of tidal dissipation is 1 or 2 orders of magnitude weaker. As the WASP-18 system is one of the prime candidates for detection of orbital decay, further timing observations are expected to push the boundaries of our knowledge on stellar interiors.

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**ISSN:** 0001-5237

#### Record 12 of 236

**Title:** Improved Cation Binding to Lipid Bilayers with Negatively Charged POPS by Effective Inclusion of Electronic Polarization

**Author(s):** Melcr, J (Melcr, Josef); Ferreira, TM (Ferreira, Tiago M.); Jungwirth, P (Jungwirth, Pavel); Ollila, OHS (Ollila, O. H. Samuli)

**Source:** JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 16 **Issue:** 1 **Pages:** 738-748 **DOI:** 10.1021/acs.jctc.9b00824 **Published:** JAN 2020

**Abstract:** Phosphatidylserine (PS) lipids are important signaling molecules and the most common negatively charged lipids in eukaryotic membranes. The signaling can be often regulated by calcium, but its interactions with PS headgroups are not fully understood. Classical molecular dynamics (MD) simulations can potentially give detailed description of lipid-ion interactions, but the results strongly depend on the used force field. Here, we apply the electronic continuum correction (EGG) to the Amber Lipid17 parameters of 1-palmitoyl-2-oleoyl-sn-glycerol-3-phospho-L-serine (POPS) lipid to improve its interactions with K<sup>+</sup>, Na<sup>+</sup>, and Ca<sup>2+</sup> ions. The partial charges of the headgroup, glycerol backbone, and carbonyls of POPS, bearing a unit negative charge, were scaled with a factor of 0.75, derived for monovalent ions, and the Lennard-Jones sigma parameters of the same segments were scaled with a factor of 0.89. The resulting ECC-POPS model gives more realistic interactions with Na<sup>+</sup> and Ca<sup>2+</sup> cations than the original Amber Lipid17 parameters when validated using headgroup order parameters and the "electrometer concept". In ECC-lipids simulations, populations of complexes of Ca<sup>2+</sup> cations with more than two PS lipids are negligible, and interactions of Ca<sup>2+</sup> cations with only carboxylate groups are twice more likely than with only phosphate groups, while interactions with carbonyls almost entirely involve other groups as well. Our results pave the way for more realistic MD simulations of biomolecular systems with anionic membranes, allowing signaling processes involving PS and Ca<sup>2+</sup> to be elucidated.

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**PubMed ID:** 31762275

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Ollila, Samuli	C-9453-2013	0000-0002-8728-1006
Jungwirth, Pavel	D-9290-2011	0000-0002-6892-3288
Melcr, Josef	G-8562-2014	0000-0003-4729-3990

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#### Record 13 of 236

**Title:** Energy components in energy decomposition analysis (EDA) are path functions; why does it matter?

**Author(s):** Andrada, DM (Andrada, Diego M.); Foroutan-Nejad, C (Foroutan-Nejad, Cina)

**Source:** PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 22 **Issue:** 39 **Pages:** 22459-22464 **DOI:** 10.1039/d0cp04016a **Published:** OCT 21 2020

**Abstract:** Here, we discuss that unlike bond dissociation energy (BDE) that is a state function quantity, the energy components of the energy decomposition analysis (EDA), i.e. electrostatic interaction, Pauli repulsion, and orbital interaction, are path (process) function quantities. Being a path function means that EDA energy components are not uniquely defined, i.e. the relative magnitudes of the orbital interaction, Pauli repulsion, and electrostatic components may vary depending on the selected pathway for EDA. Therefore, at best, EDA can define whether closely related chemical bonds are more or less ionic/covalent compared with each other. However, a precise assessment of the nature of a certain type of chemical bond using EDA is a questionable task. Besides, we briefly discuss that the widely used EDA pathway, which is merely an arbitrary choice among infinite possible paths, comes to conclusions not consistent with our widely accepted knowledge of bond formation even for the simplest molecules.

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**PubMed ID:** 32996940

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173

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#### Record 14 of 236

**Title:** Kitaev Spin Liquid in 3d Transition Metal Compounds

**Author(s):** Liu, HM (Liu, Huimei); Chaloupka, J (Chaloupka, Jiri); Khaliullin, G (Khaliullin, Giniyat)

**Source:** PHYSICAL REVIEW LETTERS **Volume:** 125 **Issue:** 4 **Article Number:** 047201 **DOI:** 10.1103/PhysRevLett.125.047201 **Published:** JUL 21 2020

**Abstract:** We study the exchange interactions and resulting magnetic phases in the honeycomb cobaltates. For a broad range of trigonal crystal fields acting on Co<sup>2+</sup> ions, the low-energy pseudospin-1/2 Hamiltonian is dominated by bond-dependent Ising couplings that constitute the Kitaev model. The non-Kitaev terms nearly vanish at small values of trigonal field Delta, resulting in spin liquid ground state. Considering Na<sub>3</sub>Co<sub>2</sub>SbO<sub>6</sub> as an example, we find that this compound is proximate to a Kitaev spin liquid phase, and can be driven into it by slightly reducing Delta by similar to 20 meV, e.g., via strain or pressure control. We argue that, due to the more localized nature of the magnetic electrons in 3d compounds, cobaltates offer the most promising search area for Kitaev model physics.

**Accession Number:** WOS:000550580800010

**PubMed ID:** 32794780

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Chaloupka, Jiri		0000-0001-8898-0442

**ISSN:** 0031-9007

**eISSN:** 1079-7114

#### Record 15 of 236

**Title:** A study on interwoven hydrogen bonding interactions in new zidovudine-picric acid (1:1) cocrystal through single crystal XRD, spectral and computational methods

**Author(s):** Likhitha, U (Likhitha, U.); Narayana, B (Narayana, B.); Sarojini, BK (Sarojini, B. K.); Kumar, SM (Kumar, S. Madan); Lobo, AG (Lobo, Anupam G.); Karthick, T (Karthick, T.)

**Source:** JOURNAL OF MOLECULAR STRUCTURE **Volume:** 1211 **Article Number:** 128052 **DOI:** 10.1016/j.molstruc.2020.128052 **Published:** JUL 5 2020

**Abstract:** High throughput of cocrystals furnishes information on the proximity of an Active Pharmaceutical Ingredient (API) and cofomer. In this paper, the mechanochemical synthesis of 1:1 cocrystal of anti-HIV drug Zidovudine (AZT), with Picric acid (PA) is presented. The single-crystal X-ray diffraction confirms that cocrystal is crystallized in the monoclinic crystal system (space group P21) with one molecule of AZT and a molecule of PA in the asymmetric unit. The molecular interactions in the crystal structure were analyzed by considering short contacts and intermolecular contacts using quantum topological atoms in molecules (QTAIM) and Hirshfeld surface methods. In the crystal structure of AZT-PA, intermolecular hydrogen bonds (N-H center dot center dot center dot O, O-H center dot center dot center dot O, C-H center dot center dot center dot O, and C-H center dot center dot center dot pi) were involved in the formation of supramolecular assembly. The major inter contacts O center dot center dot center dot H and N center dot center dot center dot H contribute 38.4% and 11.1% respectively as resulted from Hirshfeld Surfaces. The cocrystal models were illustrated using density functional theory and the quantum topology. The experimental and theoretical FTIR spectrum of the cocrystal was compared and analyzed. Also, the crystal packing was analyzed using molecular dynamics (supercell model). Additionally, Thermoanalytical methods (DSC/TGA) indicated that the crystallinity of AZT-PA was preserved up to 129 degrees C. (C) 2020 Elsevier B.V. All rights reserved.

**Accession Number:** WOS:000526086200002

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
T., karthick		0000-0001-6029-8644
Lobo, Anupam Glorious	L-8691-2016	0000-0002-0883-3715

**ISSN:** 0022-2860



eISSN: 1872-8014

## Record 16 of 236

**Title:** Molecular dynamics and experimental study of the growth, structure and properties of Zr-Cu films**Author(s):** Houska, J (Houska, Jiri); Machanova, P (Machanova, Pavla); Zitek, M (Zitek, Michal); Zeman, P (Zeman, Petr)**Source:** JOURNAL OF ALLOYS AND COMPOUNDS **Volume:** 828 **Article Number:** 154433 **DOI:** 10.1016/j.jallcom.2020.154433 **Published:** JUL 5 2020**Abstract:** Extensive molecular dynamics simulations of the atom-by-atom growth of Zr-Cu films were performed in a wide range of compositions, energies and growth templates. The results are correlated with and used to explain experimental results obtained using magnetron sputtering of the same films. After the identification of compositional ranges corresponding to crystalline and amorphous films, we particularly focus on the evolution of characteristics of the amorphous compositions. The quantities of interest include resputtering during the film growth, surface composition, densification, crystallinity, homogeneity, short-range order (bonding statistics and coordination numbers), medium-range order (ring statistics and common neighbor statistics) and functional properties (hardness and glass transition temperature). The results are important for understanding the structures and properties of Zr-Cu films in general and Zr-Cu metallic glasses in particular, and for the design of pathways for their preparation. (c) 2020 Elsevier B.V. All rights reserved.**Accession Number:** WOS:000522634300060**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Houska, Jiri	B-9616-2016	0000-0002-4809-4128
Zeman, Petr	B-9252-2016	0000-0001-8742-4487
Zitek, Michal		0000-0001-8962-7675

ISSN: 0925-8388

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## Record 17 of 236

**Title:** Atomic Charge Calculator II: web-based tool for the calculation of partial atomic charges**Author(s):** Racek, T (Racek, Tomas); Schindler, O (Schindler, Ondrej); Tousek, D (Tousek, Dominik); Horsky, V (Horsky, Vladimir); Berka, K (Berka, Karel); Koca, J (Koca, Jaroslav); Svobodova, R (Svobodova, Radka)**Source:** NUCLEIC ACIDS RESEARCH **Volume:** 48 **Issue:** W1 **Pages:** W591-W596 **DOI:** 10.1093/nar/gkaa367 **Published:** JUL 2 2020**Abstract:** Partial atomic charges serve as a simple model for the electrostatic distribution of a molecule that drives its interactions with its surroundings. Since partial atomic charges are frequently used in computational chemistry, chemoinformatics and bioinformatics, many computational approaches for calculating them have been introduced. The most applicable are fast and reasonably accurate empirical charge calculation approaches. Here, we introduce Atomic Charge Calculator II (ACC II), a web application that enables the calculation of partial atomic charges via all the main empirical approaches and for all types of molecules. ACC II implements 17 empirical charge calculation methods, including the highly cited (QEq, EEM), the recently published (EQeq, EQeq+C), and the old but still often used (PEOE). ACC II enables the fast calculation of charges even for large macromolecular structures. The web server also offers charge visualization, courtesy of the powerful LiteMol viewer. The calculation setup of ACC II is very straightforward and enables the quick calculation of high-quality partial charges. The application is available at <https://acc2.ncbr.muni.cz>.**Accession Number:** WOS:000562474100079**PubMed ID:** 32402071**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Svobodova, Radka	E-2867-2012	
report, for	ABC-8303-2020	0000-0002-3840-8760
Berka, Karel	E-2839-2010	0000-0001-9472-2589

ISSN: 0305-1048

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## Record 18 of 236

**Title:** The evolutionary origins of auxin transport: what we know and what we need to know**Author(s):** Vosolsobe, S (Vosolsobe, Stanislav); Skokan, R (Skokan, Roman); Petrasek, J (Petrasek, Jan)**Source:** JOURNAL OF EXPERIMENTAL BOTANY **Volume:** 71 **Issue:** 11 **Pages:** 3287-3295 **DOI:** 10.1093/jxb/eraa169 **Published:** JUN 11 2020**Abstract:** Auxin, represented by indole-3-acetic acid (IAA), has for a long time been studied mainly with respect to the development of land plants, and recent evidence confirms that canonical nuclear auxin signaling is a land plant apomorphy. Increasing sequential and physiological data show that the presence of auxin transport machinery pre-dates the emergence of canonical signaling. In this review, we summarize the present state of knowledge regarding the origins of auxin transport in the green lineage (Viridiplantae), integrating both data from wet lab experiments and sequence evidence on the presence of PIN-FORMED (PIN), PIN-LIKES (PILS), and AUXIN RESISTANT 1/LIKE-AUX1 (AUX1/LAX) homologs. We discuss a high divergence of auxin carrier homologs among algal lineages and emphasize the urgent need for the establishment of good molecular biology models from within the streptophyte green algae. We further postulate and discuss two hypotheses for the ancestral role of auxin in the green lineage. First, auxin was present as a by-product of cell metabolism and the evolution of its transport was stimulated by the need for IAA sequestration and cell detoxification. Second, auxin was primarily a signaling compound, possibly of bacterial origin, and its activity in the pre-plant green algae was a consequence of long-term co-existence with bacteria in shared ecological consortia.**Accession Number:** WOS:000544177200006**PubMed ID:** 32246155**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Vosolsobe, Stanislav	H-9104-2017	0000-0002-1180-3250
Petrasek, Jan	C-8240-2009	0000-0002-6719-2735
Skokan, Roman		0000-0003-0467-0792

ISSN: 0022-0957

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## Record 19 of 236

**Title:** Crystal time-reversal symmetry breaking and spontaneous Hall effect in collinear antiferromagnets**Author(s):** Smejkal, L (Smejkal, Libor); Gonzalez-Hernandez, R (Gonzalez-Hernandez, Rafael); Jungwirth, T (Jungwirth, T.); Sinova, J (Sinova, J.)**Source:** SCIENCE ADVANCES **Volume:** 6 **Issue:** 23 **Article Number:** eaaz8809 **DOI:** 10.1126/sciadv.aaz8809 **Published:** JUN 2020**Abstract:** Electrons, commonly moving along the applied electric field, acquire in certain magnets a dissipationless transverse velocity. This spontaneous Hall effect, found more than a century ago, has been understood in terms of the time-reversal symmetry breaking by the internal spin structure of a ferromagnetic, noncollinear anti-ferromagnetic, or skyrmionic form. Here, we identify previously overlooked robust Hall effect mechanism arising from collinear antiferromagnetism combined with nonmagnetic atoms at noncentrosymmetric positions. We predict a large magnitude of this crystal Hall effect in a room temperature collinear antiferromagnet RuO<sub>2</sub> and catalog, based on symmetry rules, extensive families of material candidates. We show that the crystal Hall effect is accompanied by the possibility to control its sign by the crystal chirality. We illustrate that accounting for the full magnetization density distribution instead of the simplified spin structure sheds new light on symmetry breaking phenomena in magnets and opens an alternative avenue toward low-dissipation nanoelectronics.**Accession Number:** WOS:000540787200025**PubMed ID:** 32548264**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Gonzalez-Hernandez, Rafael	A-4977-2013	0000-0003-1761-4116
Jungwirth, Tomas	G-8952-2014	0000-0002-9910-1674

ISSN: 2375-2548

## Record 20 of 236

**Title:** Magnetic properties of Mn-doped Bi<sub>2</sub>Se<sub>3</sub> topological insulators: Ab initio calculations

**Author(s):** Carva, K (Carva, K.); Balaz, P (Balaz, P.); Sebesta, J (Sebesta, J.); Turek, I (Turek, I.); Kudrnovsky, J (Kudrnovsky, J.); Maca, F (Maca, F.); Drchal, V (Drchal, V); Chico, J (Chico, J.); Sechovsky, V (Sechovsky, V); Honolka, J (Honolka, J.)

**Source:** PHYSICAL REVIEW B **Volume:** 101 **Issue:** 5 **Article Number:** 054428 **DOI:** 10.1103/PhysRevB.101.054428 **Published:** FEB 20 2020

**Abstract:** Doping Bi<sub>2</sub>Se<sub>3</sub> by magnetic ions represents an interesting problem since it may break the time-reversal symmetry needed to maintain the topological insulator character. Mn dopants in Bi<sub>2</sub>Se<sub>3</sub> represent one of the most studied examples here. However, there is a lot of open questions regarding their magnetic ordering. In the experimental literature different Curie temperatures or no ferromagnetic order at all are reported for comparable Mn concentrations. This suggests that magnetic ordering phenomena are complex and highly susceptible to different growth parameters, which are known to affect material defect concentrations. So far theory has focused on Mn dopants in one possible position, and neglected relaxation effects as well as native defects. We have used ab initio methods to calculate the Bi<sub>2</sub>Se<sub>3</sub> electronic structure influenced by magnetic Mn dopants, and exchange interactions between them. We have considered two possible Mn positions, the substitutional and interstitial one, and also native defects. We have found a sizable relaxation of atoms around Mn, which affects significantly magnetic interactions. Surprisingly, very strong interactions correspond to a specific position of Mn atoms separated by a van der Waals gap. Based on the calculated data we performed spin dynamics simulations to examine systematically the resulting magnetic order for various defect contents. We have found under which conditions the experimentally measured Curie temperatures T-C can be reproduced, noticing that interstitial Mn atoms appear to be important here. Our theory predicts the change of T-C with a shift of Fermi level, which opens the way to tune the system magnetic properties by selective doping.

**Accession Number:** WOS:000514683900002

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Balaz, Pavel	M-9510-2015	0000-0003-0016-9271
Maca, Frantisek	G-4467-2014	0000-0002-8004-9132
Sechovsky, Vladimir	A-5256-2008	0000-0003-1298-2120
Turek, Iija	G-5553-2014	0000-0002-0604-6590

**ISSN:** 2469-9950

**eISSN:** 2469-9969

**Record 21 of 236**

**Title:** Separation of racemic compound by nanofibrous composite membranes with chiral selector

**Author(s):** Gaalova, J (Gaalova, Jana); Yalcinkaya, F (Yalcinkaya, Fatma); Curinova, P (Curinova, Petra); Kohout, M (Kohout, Michal); Yalcinkaya, B (Yalcinkaya, Baturalp); Kostejn, M (Kostejn, Martin); Jirsak, J (Jirsak, Jan); Stibor, I (Stibor, Ivan); Bara, JE (Bara, Jason E.); Van der Bruggen, B (Van der Bruggen, Bart); Izak, P (Izak, Pavel)

**Source:** JOURNAL OF MEMBRANE SCIENCE **Volume:** 596 **Article Number:** 117728 **DOI:** 10.1016/j.memsci.2019.117728 **Published:** FEB 15 2020

**Abstract:** A series of unique composite membranes formed from a nano-fibrous material with different amounts of a chiral selector was used for separation of chiral drugs. The membrane performances were demonstrated through sorption tests, wherein they were soaked in an aqueous solution of racemic D, L-tryptophan (a model chiral drug). The changes in concentration of both enantiomers over time were monitored by HPLC analysis. During 100 days, a blank membrane (without the chiral selector) exhibited no sorption activity. The membranes containing the selector had no influence on the amount of D-enantiomer, while the L-enantiomer was preferentially adsorbed on each membrane. The intensity of the sorption was found to be a direct function of the amount of the selector contained in a particular membrane. The separation of the same model chiral compound was further studied in diffusion cells by pertraction. The preferential sorption of L-tryptophan in the feed underlined the crucial importance of the selector in an active layer in view of chiral recognition of enantiomers. Due to the exclusive membrane material, the retention of L-tryptophan in the membrane materials did not block the passage of D-enantiomer into the permeate at any point during the experiment. Moreover, the nanomaterial in the active layer assured the distribution of the selector to the point that only 50% of (S, S)-1,2-diaminocyclohexane in one part of the active layer was sufficient to achieve 99% of enantioselectivity. The membranes - fresh and used - were analysed by Fourier-transform infrared (FTIR) spectroscopy and characterized by scanning electron microscopy (SEM) confirming the stability of the tested membranes. To complete the study, the role of the polyamide active layer in chiral recognition of tryptophan enantiomers was proposed.

**Accession Number:** WOS:000512677400041

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Gaalova, Jana	AAR-2780-2020	0000-0002-9060-5200
Kohout, Michal	R-7707-2016	0000-0003-1447-4453
Van der Bruggen, Bart	AAR-3676-2020	
Yalcinkaya, Fatma	A-2141-2014	0000-0002-5057-3718
Jirsak, Jan	A-7434-2013	0000-0003-4833-503X
Yalcinkaya, Baturalp	ABG-1511-2020	
Bara, Jason		0000-0002-8351-2145
Curinova, Petra		0000-0001-8264-7032

**ISSN:** 0376-7388

**eISSN:** 1873-3123

**Record 22 of 236**

**Title:** First-principles study of Zn-doping effects on phase stability and magnetic anisotropy of Ni-Mn-Ga alloys

**Author(s):** Janovec, J (Janovec, Jozef); Straka, L (Straka, Ladislav); Sozinov, A (Sozinov, Alexei); Heczko, O (Heczko, Oleg); Zeleny, M (Zeleny, Martin)

**Source:** MATERIALS RESEARCH EXPRESS **Volume:** 7 **Issue:** 2 **Article Number:** 026101 **DOI:** 10.1088/2053-1591/ab6925 **Published:** FEB 2020

**Abstract:** The effect of Zn doping on Ni-Mn-Ga magnetic shape memory alloy was studied by the first-principles calculations using exact muffin-tin orbital method in combination with the coherent-potential approximation and projector augmented-wave method. Trends in martensitic transformation temperature T-M and Curie temperature T-C were predicted from calculated energy differences between austenite and nonmodulated martensite, Delta EA-NM, and energy differences between paramagnetic and ferromagnetic state, Delta EPM-FM. Doping upon the Ga-sublattice results in stabilization of martensitic phase which indicates the increase in T-M. T-C is affected only weakly or slightly decreases, because Delta EPM-FM of martensite does not change significantly with doping. The substitution of Mn atoms by Zn causes the decrease in both T-M and T-C. Comparing to Cu-doped Ni-Mn-Ga alloys, we predict that doping with Zn results in smaller decrease in T-C but also in smaller increase in T-M. Moreover, Cu doping upon the Ga-sublattice strongly decreases the magnetic anisotropy energy of martensite, whereas such strong effect was not observed for Zn doping. Based on the calculations of Zn-doped Ni-Mn-Ga alloys we suggest that simultaneous doping with Zn and an element increasing T-C can result in significant increase in both transformation temperatures without strong decrease of magnetic anisotropy.

**Accession Number:** WOS:000525697600001

**Author Identifiers:**

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

**eISSN:** 2053-1591

**Record 23 of 236**

**Title:** Evolutionary history and genetic diversity of apomictic allopolyploids in Hieracium s.str.: morphological versus genomic features

**Author(s):** Chrtek, J (Chrtek, Jindrich); Mraz, P (Mraz, Patrik); Belyayev, A (Belyayev, Alexander); Pastova, L (Pastova, Ladislava); Mrázová, V (Mrázová, Viera); Caklova, P (Caklova, Petra); Josefičová, J (Josefičová, Jirina); Zagorski, D (Zagorski, Danijela); Hartmann, M (Hartmann, Matthias); Jandova, M (Jandova, Michaela); Pinc, J (Pinc, Jan); Fehrer, J (Fehrer, Judith)

**Source:** AMERICAN JOURNAL OF BOTANY **Volume:** 107 **Issue:** 1 **Pages:** 66-90 **DOI:** 10.1002/ajb2.1413 **Early Access Date:** JAN 2020 **Published:** JAN 2020

**Abstract:** Premise The origin of allopolyploids is believed to shape their evolutionary potential, ecology, and geographical ranges. Morphologically distinct apomictic types sharing the same parental species belong to the most challenging groups of polyploids. We evaluated the origins and variation of two triploid taxa (*Hieracium pallidiflorum*, *H. picroides*) presumably derived from the same diploid parental pair (*H. intybaceum*, *H. prenanthoides*). Methods We used a suite of approaches ranging from morphological, phylogenetic (three unlinked molecular markers), and cytogenetic analyses (in situ hybridization) to genome size screening and genome skimming. Results Genotyping proved the expected parentage of all analyzed accessions of *H. pallidiflorum* and *H. picroides* and revealed that nearly all of them originated independently. Genome sizes and genome dosage largely corresponded to morphology, whereas the maternal origin of the allopolyploids had no discernable effect. Polyploid accessions of both parental species usually contained genetic material from other species. Given the phylogenetic distance of the parents, their chromosomes appeared only weakly differentiated in genomic in situ hybridization (GISH), as well as in overall comparisons of the repetitive fraction of their genomes. Furthermore, the repeatome of a phylogenetically more closely related species (*H. umbellatum*) differed significantly more. Conclusions We proved (1) multiple origins of hybridogeneous apomicts from the same diploid parental taxa, and (2) allopolyploid origins of polyploid accessions of the parental species. We also showed that the evolutionary dynamics of very fast evolving markers such as satellite DNA or transposable elements does not necessarily follow patterns of speciation.

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PubMed ID: 31903548

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Mraz, Patrik	ABD-9484-2020	0000-0002-1415-070X
Belyayev, Alexander	G-1611-2014	0000-0002-8933-6197
Mraz, Patrik	I-5965-2016	0000-0002-1415-070X
Fehrer, Judith	B-9296-2013	0000-0002-0337-5444

ISSN: 0002-9122

eISSN: 1537-2197

**Record 24 of 236****Title:** Influence of Terminal Carboxyl Groups on the Structure and Reactivity of Functionalized m-Carboranethiolate Self-Assembled Monolayers**Author(s):** Goronzy, DP (Goronzy, Dominic P.); Stanek, J (Stanek, Jan); Avery, E (Avery, Erin); Guo, H (Guo, Han); Bastl, Z (Bastl, Zdenek); Dusek, M (Dusek, Michal); Gallup, NM (Gallup, Nathan M.); Gun, S (Gun, Saliha); Kucerakova, M (Kucerakova, Monika); Levandowski, BJ (Levandowski, Brian J.); Machacek, J (Machacek, Jan); Sicha, V (Sicha, Vaclav); Thomas, JC (Thomas, John C.); Yavuz, A (Yavuz, Adem); Houk, KN (Houk, K. N.); Danisman, MF (Danisman, Mehmet Fatih); Mete, E (Mete, Ersen); Alexandrova, AN (Alexandrova, Anastassia N.); Base, T (Base, Tomas); Weiss, PS (Weiss, Paul S.)**Source:** CHEMISTRY OF MATERIALS **Volume:** 32 **Issue:** 15 **Pages:** 6800-6809 **DOI:** 10.1021/acs.chemmater.0c02722 **Published:** AUG 11 2020**Abstract:** The structure and function of self-assembled monolayers (SAMs) at the nanoscale are determined by the steric and electronic effects of their building blocks. Carboranethiol molecules form pristine monolayers that provide tunable two-dimensional systems to probe lateral and interfacial interactions. Additional omega-functionality, such as carboxyl groups, can be introduced to change the properties of the exposed surfaces. Here, two geometrically similar isomeric m-carborane analogues of m-mercaptobenzoic acid, 1-COOH-7-SH-1,7-C2B10H10 and racem-1-COOH-9-SH-1,7-C2B10H10, are characterized and their SAMs on Au(111) are examined. The latter isomer belongs to the rare group of chiral cage molecules and becomes, to our knowledge, the first example assembled on Au(111). Although different in symmetry, molecules of both isomers assemble into similar hexagonal surface patterns. The nearest-neighbor spacing of 8.4 +/- 0.4 angstrom is larger than that of non-carboxylated isomers, consistent with the increased steric demands of the carboxyl groups. Computational modeling reproduced this spacing and suggests a tilt relative to the surface normal. However, tilt domains are not observed experimentally, suggesting the presence of strong lateral interactions. Analyses of the influence of the functional groups through the pseudo-aromatic m-carborane skeleton showed that the thiol group attached to either carbon or boron atoms increases the carboxyl group acidity in solution. In contrast, the acidity of the exposed carboxyl group in the SAMs decreases upon surface attachment; computational analyses suggest that the driving force of this shift is the dielectric of the environment in the monolayer as a result of confined intermolecular interactions, proximity to the Au surface, and partial desolvation.**Accession Number:** WOS:000562136900054

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Danisman, Mehmet Fatih	AAZ-6619-2020	
Weiss, Paul S	A-2575-2011	0000-0001-5527-6248
Mete, Ersen	G-7002-2018	0000-0002-0916-5616
Dusek, Michal	B-7316-2011	0000-0001-9797-2559

ISSN: 0897-4756

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**Record 25 of 236****Title:** EnzymeMiner: automated mining of soluble enzymes with diverse structures, catalytic properties and stabilities**Author(s):** Hon, J (Hon, Jiri); Borko, S (Borko, Simeon); Stourac, J (Stourac, Jan); Prokop, Z (Prokop, Zbynek); Zendulka, J (Zendulka, Jaroslav); Bednar, D (Bednar, David); Martinek, T (Martinek, Tomas); Damborsky, J (Damborsky, Jiri)**Source:** NUCLEIC ACIDS RESEARCH **Volume:** 48 **Issue:** W1 **Pages:** W104-W109 **DOI:** 10.1093/nar/gkaa372 **Published:** JUL 2 2020**Abstract:** Millions of protein sequences are being discovered at an incredible pace, representing an inexhaustible source of biocatalysts. Despite genomic databases growing exponentially, classical biochemical characterization techniques are time-demanding, cost-ineffective and low-throughput. Therefore, computational methods are being developed to explore the unmapped sequence space efficiently. Selection of putative enzymes for biochemical characterization based on rational and robust analysis of all available sequences remains an unsolved problem. To address this challenge, we have developed EnzymeMiner—a web server for automated screening and annotation of diverse family members that enables selection of hits for wet-lab experiments. EnzymeMiner prioritizes sequences that are more likely to preserve the catalytic activity and are heterologously expressible in a soluble form in Escherichia coli. The solubility prediction employs the in-house SoluProt predictor developed using machine learning. EnzymeMiner reduces the time devoted to data gathering, multi-step analysis, sequence prioritization and selection from days to hours. The successful use case for the haloalkane dehalogenase family is described in a comprehensive tutorial available on the EnzymeMiner web page.**Accession Number:** WOS:000562474100017

PubMed ID: 32392342

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Bednar, David	ABF-5943-2020	0000-0002-6803-0340
Hon, Jiri		0000-0002-3321-9629
Damborsky, Jiri	H-3799-2012	0000-0002-7848-8216

ISSN: 0305-1048

eISSN: 1362-4962

**Record 26 of 236****Title:** A benchmark set of highly-efficient CUDA and OpenCL kernels and its dynamic autotuning with Kernel Tuning Toolkit**Author(s):** Petrovic, F (Petrovic, Filip); Strelak, D (Strelak, David); Hozzova, J (Hozzova, Jana); Ol'ha, J (Ol'ha, Jaroslav); Trembecky, R (Trembecky, Richard); Benkner, S (Benkner, Siegfried); Filipovic, J (Filipovic, Jiri)**Source:** FUTURE GENERATION COMPUTER SYSTEMS-THE INTERNATIONAL JOURNAL OF ESCIENCE **Volume:** 108 **Pages:** 161-177 **DOI:** 10.1016/j.future.2020.02.069 **Published:** JUL 2020**Abstract:** In recent years, the heterogeneity of both commodity and supercomputers hardware has increased sharply. Accelerators, such as GPUs or Intel Xeon Phi co-processors, are often key to improving speed and energy efficiency of highly-parallel codes. However, due to the complexity of heterogeneous architectures, optimization of codes for a certain type of architecture as well as porting codes across different architectures, while maintaining a comparable level of performance, can be extremely challenging. Addressing the challenges associated with performance optimization and performance portability, autotuning has gained a lot of interest. Autotuning of performance-relevant source-code parameters allows to automatically tune applications without hard coding optimizations and thus helps with keeping the performance portable. In this paper, we introduce a benchmark set of ten autotunable kernels for important computational problems implemented in OpenCL or CUDA. Using our Kernel Tuning Toolkit, we show that with autotuning most of the kernels reach near-peak performance on various GPUs and outperform baseline implementations on CPUs and Xeon Phis. Our evaluation also demonstrates that autotuning is key to performance portability. In addition to offline tuning, we also introduce dynamic autotuning of code optimization parameters during application runtime. With dynamic tuning, the Kernel Tuning Toolkit enables applications to re-tune performance-critical kernels at runtime whenever needed, for example, when input data changes. Although it is generally believed that autotuning spaces tend to be too large to be searched during application runtime, we show that it is not necessarily the case when tuning spaces are designed rationally. Many of our kernels reach near peak-performance with moderately sized tuning spaces that can be searched at runtime with acceptable overhead. Finally we demonstrate, how dynamic performance tuning can be integrated into a real-world application from cryo-electron microscopy domain. (C) 2020 Elsevier B.V. All rights reserved.**Accession Number:** WOS:000528199900012

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Filipovic, Jiri	H-4311-2013	0000-0002-5703-9673

ISSN: 0167-739X



eISSN: 1872-7115

## Record 27 of 236

**Title:** Molecular Insights into the Architecture of the Human SMC5/6 Complex**Author(s):** Adamus, M (Adamus, M.); Lelkes, E (Lelkes, E.); Potesil, D (Potesil, D.); Ganji, SR (Ganji, S. R.); Kolesar, P (Kolesar, P.); Zabradny, K (Zabradny, K.); Zdrahal, Z (Zdrahal, Z.); Palecek, JJ (Palecek, J. J.)**Source:** JOURNAL OF MOLECULAR BIOLOGY **Volume:** 432 **Issue:** 13 **Pages:** 3820-3837 **DOI:** 10.1016/j.jmb.2020.04.024 **Published:** JUN 12 2020**Abstract:** A family of Structural Maintenance of Chromosome (SMC) complexes is essential for key cellular processes ensuring proper cohesion, condensation and replication. They share a common SMC-kleisin architecture allowing them to embrace DNA. In SMC5/6, the NSE1 and NSE3 KITE and NSE4 kleisin subunits form a stable subcomplex that binds DNA and regulates essential processes. In addition, NSE5 and NSE6 subunits associate with the core SMC5/6 complex and recruit it to DNA repair sites.

The architecture of the SMC5/6 complex is crucial for its proper functioning, and mutations within the human SMC5/6 subunits result in severe syndromes. Therefore, we aimed to analyze interactions within the human SMC5/6 complex and determine its detailed architecture. Firstly, we analyzed different parts of SMC5/6 by crosslinking and MS/MS analysis. Our data suggested domain arrangements of hNSE1-hNSE3 and orientation of hNSE4 within the hNSE1-hNSE3-hNSE4 subcomplex. The crosslinking and electron microscopic analysis of the SMC5/6 core complex showed its rod-like architecture with juxtaposed hSMC5-hSMC6 arms. Additionally, we observed fully or partially opened hSMC5-hSMC6 shapes with the hNSE1-hNSE3-hNSE4 trimer localized in the SMC head domains. To complete mapping of the human SMC5/6 complex architecture, we analyzed positions of hNSE5-hNSE6 at the hSMC5-hSMC6 arms. We showed that hNSE6 binding to hNSE5 and the coiled-coil arm of hSMC6 is mediated by a conserved FAM178 domain, which we therefore renamed CANIN (Coiled-coil SMC6 And NSE5 iNteracting) domain. Interestingly, hNSE6 bound both hSMC5 and hSMC6 arms, suggesting that hNSE6 may lock the arms and regulate the dynamics of the human SMC5/6 complex. (C) 2020 Elsevier Ltd. All rights reserved.

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Author	Web of Science ResearcherID	ORCID Number
Adamus, Marek	AAR-1543-2020	0000-0003-0520-745X
Palecek, Jan	D-6864-2012	0000-0002-6223-5169

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## Record 28 of 236

**Title:** QSAR-derived affinity fingerprints (part 2): modeling performance for potency prediction**Author(s):** Cortes-Ciriano, I (Cortes-Ciriano, Isidro); Skuta, C (Skuta, Ctibor); Bender, A (Bender, Andreas); Svozil, D (Svozil, Daniel)**Source:** JOURNAL OF CHEMINFORMATICS **Volume:** 12 **Issue:** 1 **Article Number:** 41 **DOI:** 10.1186/s13321-020-00444-5 **Published:** JUN 5 2020**Abstract:** Affinity fingerprints report the activity of small molecules across a set of assays, and thus permit to gather information about the bioactivities of structurally dissimilar compounds, where models based on chemical structure alone are often limited, and model complex biological endpoints, such as human toxicity and in vitro cancer cell line sensitivity. Here, we propose to model in vitro compound activity using computationally predicted bioactivity profiles as compound descriptors. To this aim, we apply and validate a framework for the calculation of QSAR-derived affinity fingerprints (QAFFP) using a set of 1360 QSAR models generated using K-i, K-d, IC50 and EC50 data from ChEMBL database. QAFFP thus represent a method to encode and relate compounds on the basis of their similarity in bioactivity space. To benchmark the predictive power of QAFFP we assembled IC50 data from ChEMBL database for 18 diverse cancer cell lines widely used in preclinical drug discovery, and 25 diverse protein target data sets. This study complements part 1 where the performance of QAFFP in similarity searching, scaffold hopping, and bioactivity classification is evaluated. Despite being inherently noisy, we show that using QAFFP as descriptors leads to errors in prediction on the test set in the similar to 0.65-0.95 pIC(50) units range, which are comparable to the estimated uncertainty of bioactivity data in ChEMBL (0.76-1.00 pIC(50) units). We find that the predictive power of QAFFP is slightly worse than that of Morgan2 fingerprints and 1D and 2D physicochemical descriptors, with an effect size in the 0.02-0.08 pIC(50) units range. Including QSAR models with low predictive power in the generation of QAFFP does not lead to improved predictive power. Given that the QSAR models we used to compute the QAFFP were selected on the basis of data availability alone, we anticipate better modeling results for QAFFP generated using more diverse and biologically meaningful targets. Data sets and Python code are publicly available at.**Accession Number:** WOS:000549151400001**PubMed ID:** 33431016**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Svozil, Daniel		0000-0003-2577-5163
Cortes Ciriano, Isidro		0000-0002-2036-494X
Skuta, Ctibor		0000-0001-5325-4934

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## Record 29 of 236

**Title:** Dhati Welel virus, the missing mammarenavirus of the widespread *Mastomys natalensis***Author(s):** De Bellocq, JG (De Bellocq, Joelle Gouy); Bryjova, A (Bryjova, Anna); Martynov, AA (Martynov, Aleksey A.); Lavrenchenko, LA (Lavrenchenko, Leonid A.)**Source:** JOURNAL OF VERTEBRATE BIOLOGY **Volume:** 69 **Issue:** 2 **Article Number:** 20018 **DOI:** 10.25225/jvb.20018 **Published:** JUN 2020**Abstract:** The Natal multimammate mouse, *Mastomys natalensis*, occurs throughout sub-Saharan Africa. Mitochondrial phylogenetics indicate this species was fragmented during the Pleistocene, forming six matrilineage phylogroups: A-I, A-II, A-III, B-IV, B-V, B-VI with distinct ranges. All except the A-III lineage are identified as natural reservoirs of mammarenaviruses. *M. natalensis* A-III is found in western Ethiopia and is the only lineage reported in the country. While screening 203 small mammal samples from Dhati Welel National Park for mammarenaviruses, we detected mammarenavirus RNA in nine samples, eight from *M. natalensis* and one from *M. awashensis*. A sequence similarity search and phylogenetic analysis confirmed the *M. natalensis* mitochondrial DNA belongs to the A-III lineage. We characterised the complete virus genome, which showed typical mammarenavirus organisation. Phylogenetic analysis indicated it clusters with Cairo virus found in *M. natalensis* B-IV in Tanzania, while showing sufficient divergence from other mammarenaviruses to be considered as a new species, for which we proposed the name Dhati Welel. Additional sampling in the *M. natalensis* A-III phylogeographic range should help determine whether the detection of the virus in *M. awashensis* represents a local spill-over or if the virus circulates in both *Mastomys* species.**Accession Number:** WOS:000543817700003

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## Record 30 of 236

**Title:** Thermal properties of Ag@Ni core-shell nanoparticles**Author(s):** Vykoukal, V (Vykoukal, Vit); Zelenka, F (Zelenka, Frantisek); Bursik, J (Bursik, Jiri); Kana, T (Kana, Tomas); Kroupa, A (Kroupa, Ales); Pinkas, J (Pinkas, Jiri)**Source:** CALPHAD-COMPUTER COUPLING OF PHASE DIAGRAMS AND THERMOCHEMISTRY **Volume:** 69 **Article Number:** 101741 **DOI:** 10.1016/j.calphad.2020.101741 **Published:** JUN 2020**Abstract:** We synthesized Ag@Ni core-shell nanoparticles by the solvothermal hot injection method and characterized them as for their shape and size by dynamic light scattering (DLS), small-angle X-ray scattering (SAXS), and transmission electron microscopy (TEM). We previously demonstrated their core-shell structure by scanning transmission electron microscopy with energy dispersive spectroscopy (STEM-EDS). The silver/nickel phase diagram was calculated by the CALPHAD method, and the melting points of 10, 15, and 20 nm silver nanoparticles were predicted at 930.2, 940.7, and 946.0 degrees C, respectively. We took advantage of the nickel shell to avoid silver sintering and to confirm the calculated melting point depression (MPD). The results obtained from the differential scanning calorimetry (DSC) experiments revealed the melting points of 11-15 nm nanoparticles at 944-949 degrees C in agreement with calculated values.**Accession Number:** WOS:000535967900007

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## Record 31 of 236

**Title:** QSAR-derived affinity fingerprints (part 1): fingerprint construction and modeling performance for similarity searching, bioactivity classification and scaffold hopping**Author(s):** Skuta, C (Skuta, C.); Cortes-Ciriano, I (Cortes-Ciriano, I); Dehaen, W (Dehaen, W.); Kriz, P (Kriz, P.); van Westen, GJP (van Westen, G. J. P.); Tetko, IV (Tetko, I., V.); Bender, A (Bender, A.); Svozil, D (Svozil, D.)**Source:** JOURNAL OF CHEMINFORMATICS **Volume:** 12 **Issue:** 1 **Article Number:** 39 **DOI:** 10.1186/s13321-020-00443-6 **Published:** MAY 29 2020

**Abstract:** An affinity fingerprint is the vector consisting of compound's affinity or potency against the reference panel of protein targets. Here, we present the QAFFP fingerprint, 440 elements long in silico QSAR-based affinity fingerprint, components of which are predicted by Random Forest regression models trained on bioactivity data from the ChEMBL database. Both real-valued (rv-QAFFP) and binary (b-QAFFP) versions of the QAFFP fingerprint were implemented and their performance in similarity searching, biological activity classification and scaffold hopping was assessed and compared to that of the 1024 bits long Morgan2 fingerprint (the RDKit implementation of the ECFP4 fingerprint). In both similarity searching and biological activity classification, the QAFFP fingerprint yields retrieval rates, measured by AUC (similar to 0.65 and similar to 0.70 for similarity searching depending on data sets, and similar to 0.85 for classification) and EF5 (similar to 4.67 and similar to 5.82 for similarity searching depending on data sets, and similar to 2.10 for classification), comparable to that of the Morgan2 fingerprint (similarity searching AUC of similar to 0.57 and similar to 0.66, and EF5 of similar to 4.09 and similar to 6.41, depending on data sets, classification AUC of similar to 0.87, and EF5 of similar to 2.16). However, the QAFFP fingerprint outperforms the Morgan2 fingerprint in scaffold hopping as it is able to retrieve 1146 out of existing 1749 scaffolds, while the Morgan2 fingerprint reveals only 864 scaffolds.

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**PubMed ID:** 33431038

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Tetko, Igor V.	B-1540-2010	0000-0002-6855-0012
Kriz, Pavel		0000-0001-5773-9541
Dehaen, Wim		0000-0002-9597-0629
Cortez Ciriano, Isidro		0000-0002-2036-494X
Svozil, Daniel		0000-0003-2577-5163
Skuta, Ctibor		0000-0001-5325-4934
van Westen, Gerard	D-7432-2011	0000-0003-0717-1817

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**Record 32 of 236**

**Title:** Tuning the Reactivity and Bonding Properties of Metal Square-Planar Complexes by the Substitution(s) on the Trans-Coordinated Pyridine Ring

**Author(s):** Dvorackova, O (Dvorackova, Olga); Chval, Z (Chval, Zdenek)

**Source:** ACS OMEGA **Volume:** 5 **Issue:** 20 **Pages:** 11768-11783 **DOI:** 10.1021/acsomega.0c01161 **Published:** MAY 26 2020

**Abstract:** The kinetics of the hydration reaction on trans-[Pt(NH3)(2)(pyrX)Cl](+) (pyr = pyridine) complexes (X = OH-, Cl-, F-, Br-, NO2-, NH2, SH-, CH3, C CH, and DMA) was studied by density functional theory calculations in the gas phase and in water solution described by the implicit polarizable continuum model method. All possible positions ortho, meta, and para of the substituent X in the pyridine ring were considered. The substitution of the pyr ligand by electron-donating X's led to the strengthening of the Pt-N1(pyrX) (Pt-N-pyrX) bond and the weakening of the trans Pt-Cl or Pt-O-w bonds. The electron-withdrawing X's have exactly the opposite effect. The strengths of these bonds can be predicted from the basicity of sigma electrons on the N-pyrX atom determined on the isolated pyrX ligand. As the pyrX ring was oriented perpendicularly with respect to the plane of the complex, the nature of the X center dot center dot center dot Cl electrostatic interaction was the decisive factor for the transition-state (TS) stabilization which resulted in the highest selectivity of ortho-substituted systems with respect to the reaction rate. Because of a smaller size of X's, the steric effects influenced less importantly the values of activation Gibbs energies Delta G(double dagger) but caused geometry changes such as the elongation of the Pt-NpyrX bonds. Substitution in the meta position led to the highest Delta G(double dagger) values for most of the X's. The changes of Delta G(double dagger) because of electronic effects were the same in the gas phase and the water solvent. However, as the water solvent dampened electrostatic interactions, 2200 and 150 times differences in the reaction rate were observed between the most and the least reactive mono-substituted complexes in the gas phase and the water solvent, respectively. An additional NO2 substitution of the pyrNO(2) ligand further decelerated the rate of the hydration reaction, but on the other hand, the poly-NH2 complexes were no more reactive than the fastest o-NH2 system. In the gas phase, the poly-X complexes showed the additivity of the substituent effects with respect to the Pt-ligand bond strengths and the ligand charges.

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**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Chval, Zdenek	D-8964-2016	0000-0003-1922-8390
Dvorackova, Olga		0000-0001-9980-6992

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**Record 33 of 236**

**Title:** Aromatic Esters of the Crinane Amaryllidaceae Alkaloid Ambelline as Selective Inhibitors of Butyrylcholinesterase

**Author(s):** Marikova, J (Marikova, Jana); Ritomska, A (Ritomska, Aneta); Korabecny, J (Korabecny, Jan); Perinova, R (Perinova, Rozalie); Al Mamun, A (Al Mamun, Abdullah); Kucera, T (Kucera, Tomas); Kohelova, E (Kohelova, Eliska); Hulcova, D (Hulcova, Daniela); Kobrlova, T (Kobrlova, Tereza); Kunes, J (Kunes, Jiri); Novakova, L (Novakova, Lucie); Cahlikova, L (Cahlikova, Lucie)

**Source:** JOURNAL OF NATURAL PRODUCTS **Volume:** 83 **Issue:** 5 **Pages:** 1359-1367 **DOI:** 10.1021/acs.jnatprod.9b00561 **Published:** MAY 22 2020

**Abstract:** A total of 20 derivatives (1-20) of the crinane-type alkaloid ambelline were synthesized. These semisynthetic derivatives were assessed for their potency to inhibit both acetylcholinesterase (AChE) and butyrylcholinesterase (BuChE). To predict central nervous system (CNS) availability, logBB was calculated, and the data correlated well with those obtained from the parallel artificial membrane permeability assay (PAMPA). All compounds should be able to permeate the blood-brain barrier (BBB) according to the obtained results. A total of 7 aromatic derivatives (5, 6, 7, 9, 10, 12, and 16) with different substitution patterns showed inhibitory potency against human serum BuChE (IC50 < 5 mu M), highlighting the three top-ranked compounds as follows: 11-O-(1-naphthoyl)ambelline (16), 11-O-(2-methylbenzoyl)ambelline (6), and 11-O-(2-methoxybenzoyl)ambelline (9) with IC50 values of 0.10 +/- 0.01, 0.28 +/- 0.02, and 0.43 +/- 0.04 mu M, respectively. Notably, derivatives 6, 7, 9, and 16 displayed selective human BuChE (hBuChE) inhibition profiles with a selectivity index > 100. The in vitro results were supported by computational studies predicting plausible binding modes of the compounds in the active sites of hBuChE.

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**PubMed ID:** 32309949

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Korabecny, Jan	J-6362-2018	0000-0001-6977-7596
Ritomska, Aneta		0000-0002-9141-2929

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**Record 34 of 236**

**Title:** Potential Application of Ionic Liquids in Pharmaceutical Dosage Forms for Small Molecule Drug and Vaccine Delivery System

**Author(s):** Uddin, M (Uddin, Mohammad); Basak, D (Basak, Debasish); Hopefl, R (Hopefl, Robert); Minofar, B (Minofar, Babak)

**Source:** JOURNAL OF PHARMACY AND PHARMACEUTICAL SCIENCES **Volume:** 23 **Pages:** 158-176 **DOI:** 10.18433/jpps30965 **Published:** MAY 10 2020

**Abstract:** Ionic liquids are salts in which the ions are poorly coordinated, which causes them to exist in liquid form below 100 degrees C, or at room temperature. Therefore, these are also defined as room temperature ionic liquids (RTILs). In ionic liquids, at least one ion has a delocalized charge and one component is organic, which prevents the formation of a stable solid form of crystal lattice. Physical properties of ionic liquids, such as melting point, viscosity, and solubility of starting materials and other solvents, are impacted by the substituents on the organic component and by the counterions. Many ionic liquids have even been developed to address specific synthetic problems and that is the reason these are also termed as "designer solvents". Ionic liquids are considered as "green solvents" that exhibit several unique characteristics such as high ionic conductivity, high solvation power, thermal stability, low volatility, and recyclability. Although very useful with several advantages, ionic liquids have some limitations that include high cost and ease of recycling. Moreover, the toxicity and biodegradability of ionic liquids are not yet well understood. Nonetheless, ionic liquids can potentially be used in the field of pharmacy in drug design and formulation development. In drug or vaccine dosage formulation development, ionic liquids can be used as a solubility enhancer, permeability enhancer, stabilizer, targeted delivery inducer, stealth property provider or bioavailability enhancer. In this article we reviewed the physical properties of ionic liquids and potential application of ionic liquids in developing formulations for vaccines and small molecule drugs (A table has been added).

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**PubMed ID:** 32407287

**ISSN:** 1482-1826

**Record 35 of 236****Title:** Toward DMRG-tailored coupled cluster method in the 4c-relativistic domain**Author(s):** Brandejs, J (Brandejs, Jan); Visnak, J (Visnak, Jakub); Veis, L (Veis, Libor); Mate, M (Mate, Mihaly); Legeza, O (Legeza, Ors); Pittner, J (Pittner, Jiri)**Source:** JOURNAL OF CHEMICAL PHYSICS **Volume:** 152 **Issue:** 17 **DOI:** 10.1063/1.5144974 **Published:** MAY 7 2020**Abstract:** There are three essential problems in computational relativistic chemistry: Electrons moving at relativistic speeds, close lying states, and dynamical correlation. Currently available quantum-chemical methods are capable of solving systems with one or two of these issues. However, there is a significant class of molecules in which all the three effects are present. These are the heavier transition metal compounds, lanthanides, and actinides with open d or f shells. For such systems, sufficiently accurate numerical methods are not available, which hinders the application of theoretical chemistry in this field. In this paper, we combine two numerical methods in order to address this challenging class of molecules. These are the relativistic versions of coupled cluster methods and the density matrix renormalization group (DMRG) method. To the best of our knowledge, this is the first relativistic implementation of the coupled cluster method externally corrected by DMRG. The method brings a significant reduction of computational costs as we demonstrate on the system of TIH, AsH, and SbH.**Accession Number:** WOS:000532172000001**PubMed ID:** 32384831**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pittner, Jiri	F-5128-2014	
Veis, Libor	F-5469-2014	0000-0002-4229-6335

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**Record 36 of 236****Title:** Evaluation of Microbiome-Host Relationships in the Zebrafish Gastrointestinal System Reveals Adaptive Immunity Is a Target of Bis(2-ethylhexyl) Phthalate (DEHP) Exposure**Author(s):** Adamovsky, O (Adamovsky, Ondrej); Buerger, AN (Buerger, Amanda N.); Vespalcova, H (Vespalcova, Hana); Sohag, SR (Sohag, Shahadur R.); Hanlon, AT (Hanlon, Amy T.); Ginn, PE (Ginn, Pamela E.); Craft, SL (Craft, Serena L.); Smatana, S (Smatana, Stanislav); Budinska, E (Budinska, Eva); Persico, M (Persico, Maria); Bisesi, JH (Bisesi, Joseph H., Jr.); Martyniuk, CJ (Martyniuk, Christopher J.)**Source:** ENVIRONMENTAL SCIENCE & TECHNOLOGY **Volume:** 54 **Issue:** 9 **Pages:** 5719-5728 **DOI:** 10.1021/acs.est.0c00628 **Published:** MAY 5 2020**Abstract:** To improve physical characteristics of plastics such as flexibility and durability, producers enrich materials with phthalates such as di-(2-ethylhexyl) phthalate (DEHP). DEHP is a high production volume chemical associated with metabolic and immune disruption in animals and humans. To reveal mechanisms implicated in phthalate-related disruption in the gastrointestinal system, male and female zebrafish were fed DEHP (3 ppm) daily for two months. At the transcriptome level, DEHP significantly upregulated gene networks in the intestine associated with helper T cells' (Th1, Th2, and Th17) specific pathways. The activation of gene networks associated with adaptive immunity was linked to the suppression of networks for tight junction, gap junctional intercellular communication, and transmembrane transporters, all of which are precursors for impaired gut integrity and performance. On a class level, DEHP exposure increased Bacteroidia and Gammaproteobacteria and decreased Verrucomicrobiae in both the male and female gastrointestinal system. Further, in males there was a relative increase in Fusobacteriia and Betaproteobacteria and a relative decrease in Saccharibacteria. Predictive algorithms revealed that the functional shift in the microbiome community, and the metabolites they produce, act to modulate intestinal adaptive immunity. This finding suggests that the gut microbiota may contribute to the adverse effects of DEHP on the host by altering metabolites sensed by both intestinal and immune Th cells. Our results suggest that the microbiome-gut-immune axis can be modified by DEHP and emphasize the value of multiomics approaches to study microbiome-host interactions following chemical perturbations.**Accession Number:** WOS:000530651900046**PubMed ID:** 32255618**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Adamovsky, Ondrej	AAW-8046-2020	0000-0003-3084-0388
Martyniuk, Christopher J.		0000-0003-0921-4796

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**Record 37 of 236****Title:** Amaryllidaceae Alkaloids of Belladine-Type from *Narcissus pseudonarcissus* cv. Carlton as New Selective Inhibitors of Butyrylcholinesterase**Author(s):** Al Mamun, A (Al Mamun, Abdullah); Marikova, J (Marikova, Jana); Hulcova, D (Hulcova, Daniela); Janousek, J (Janousek, Jiri); Safratova, M (Safratova, Marcela); Novakova, L (Novakova, Lucie); Kucera, T (Kucera, Tomas); Hrabanova, M (Hrabanova, Martina); Kunes, J (Kunes, Jiri); Korabecny, J (Korabecny, Jan); Cahlikova, L (Cahlikova, Lucie)**Source:** BIOMOLECULES **Volume:** 10 **Issue:** 5 **Article Number:** 800 **DOI:** 10.3390/biom10050800 **Published:** MAY 2020**Abstract:** Thirteen known (1-12 and 16) and three previously undescribed Amaryllidaceae alkaloids of belladine structural type, named cartonine A-C (13-15), were isolated from bulbs of *Narcissus pseudonarcissus* cv. Carlton (Amaryllidaceae) by standard chromatographic methods. Compounds isolated in sufficient amounts, and not tested previously, were evaluated for their *in vitro* acetylcholinesterase (AChE; E.C. 3.1.1.7), butyrylcholinesterase (BuChE; E.C. 3.1.1.8) and prolyl oligopeptidase (POP; E.C. 3.4.21.26) inhibition activities. Significant human BuChE (hBUChE) inhibitory activity was demonstrated by newly described alkaloids cartonine A (13) and cartonine B (14) with IC50 values of 913 +/- 20 nM and 31 +/- 1 nM, respectively. Both compounds displayed a selective inhibition pattern for hBUChE with an outstanding selectivity profile over AChE inhibition, higher than 100. The *in vitro* data were further supported by *in silico* studies of the active alkaloids 13 and 14 in the active site of hBUChE.**Accession Number:** WOS:000545013700137**PubMed ID:** 32455879**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Janousek, Jiri	T-4508-2017	0000-0002-3336-3874
Korabecny, Jan	J-6362-2018	0000-0001-6977-7596
Novakova, Lucie	S-6604-2017	0000-0003-3570-5871

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**Record 38 of 236****Title:** Nuclear inclusions of pathogenic ataxin-1 induce oxidative stress and perturb the protein synthesis machinery**Author(s):** Laidou, S (Laidou, Stamatia); Alanis-Lobato, G (Alanis-Lobato, Gregorio); Pribyl, J (Pribyl, Jan); Rasko, T (Rasko, Tamas); Tichy, B (Tichy, Boris); Mikulasek, K (Mikulasek, Kamil); Tsagiopoulou, M (Tsagiopoulou, Maria); Oppelt, J (Oppelt, Jan); Kastrinaki, G (Kastrinaki, Georgia); Lefaki, M (Lefaki, Maria); Singh, M (Singh, Manvendra); Zink, A (Zink, Annika); Chondrogianni, N (Chondrogianni, Niki); Psomopoulos, F (Psomopoulos, Fotis); Prigione, A (Prigione, Alessandro); Ivics, Z (Ivics, Zoltan); Pospisilova, S (Pospisilova, Sarka); Skladal, P (Skladal, Petr); Izsvak, Z (Izsvak, Zsuzsanna); Andrade-Navarro, MA (Andrade-Navarro, Miguel A.); Petrakis, S (Petrakis, Spyros)**Source:** REDOX BIOLOGY **Volume:** 32 **Article Number:** 101458 **DOI:** 10.1016/j.redox.2020.101458 **Published:** MAY 2020**Abstract:** Spinocerebellar ataxia type-1 (SCA1) is caused by an abnormally expanded polyglutamine (polyQ) tract in ataxin-1. These expansions are responsible for protein misfolding and self-assembly into intranuclear inclusion bodies (IIBs) that are somehow linked to neuronal death. However, owing to lack of a suitable cellular model, the downstream consequences of IIB formation are yet to be resolved. Here, we describe a nuclear protein aggregation model of pathogenic human ataxin-1 and characterize IIB effects. Using an inducible Sleeping Beauty transposon system, we overexpressed the ATXN1(Q82) gene in human mesenchymal stem cells that are resistant to the early cytotoxic effects caused by the expression of the mutant protein. We characterized the structure and the protein composition of insoluble polyQ IIBs which gradually occupy the nuclei and are responsible for the generation of reactive oxygen species. In response to their formation, our transcriptome analysis reveals a cerebellum-specific perturbed protein interaction network, primarily affecting protein synthesis. We propose that insoluble polyQ IIBs cause oxidative and nucleolar stress and affect the assembly of the ribosome by capturing or down-regulating essential components. The inducible cell system can be utilized to decipher the cellular consequences of polyQ protein aggregation. Our strategy provides a broadly applicable methodology for studying polyQ diseases.**Accession Number:** WOS:000537459900001**PubMed ID:** 32145456**Author Identifiers:**



Author	Web of Science ResearcherID	ORCID Number
Tichy, Boris	C-1314-2009	0000-0001-9252-7974
Pribyl, Jan	AA-4478-2020	
Petrakis, Spyros	AAA-6778-2021	0000-0001-9094-3480
Psomopoulos, Fotis	E-9995-2013	0000-0002-0222-4273
Tsagiopoulou, Maria		0000-0002-1653-0327
Kastrinaki, Georgia		0000-0002-0373-3117
Singh, Manvendra		0000-0002-8626-5418

ISSN: 2213-2317

**Record 39 of 236****Title:** Effect of the substituent position on the electrochemical, optical and structural properties of donor-acceptor type acridone derivatives**Author(s):** Kulszewicz-Bajer, I (Kulszewicz-Bajer, Irena); Zagorska, M (Zagorska, Malgorzata); Banasiewicz, M (Banasiewicz, Marzena); Gunka, PA (Gunka, Piotr A.); Toman, P (Toman, Petr); Kozankiewicz, B (Kozankiewicz, Boleslaw); Wiosna-Salyga, G (Wiosna-Salyga, Gabriela); Pron, A (Pron, Adam)**Source:** PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 22 Issue: 16 Pages: 8522-8534 DOI: 10.1039/d0cp00521e Published: APR 28 2020

**Abstract:** Three new donor-acceptor (D-A) compounds, positional isomers of phenoxazine-substituted acridone, namely 1-phenoxazine-N-hexylacridone (o-A), 2-phenoxazine-N-hexylacridone (m-A) and 3-phenoxazine-N-hexylacridone (p-A), were synthesized. The synthesized compounds showed interesting, isomerism-dependent electrochemistry. Their oxidation was reversible and their potential (given vs. Fc/Fc<sup>+</sup>) changed from 0.21 V for o-A to 0.36 V for p-A. In contrast, their reduction was irreversible, isomerism-independent and occurred at rather low potentials (ca. -2.25 to -2.28 V). The electrochemical results led to the following values of the ionization potentials (IPs) and electron affinities (EAs): 5.03 eV and -2.14 eV, 5.15 eV and -2.20 eV, and 5.20 eV and -2.28 eV for o-A, m-A and p-A, respectively. The experimentally obtained values were in very good agreement with those predicted by DFT calculations. All three isomers readily formed single crystals suitable for their structure determination. o-A and p-A crystallized in P1 & x304; and P2(1)/n space groups, respectively, with one molecule per asymmetric unit, while m-A crystallized in the P2(1)/c space group with two molecules in the asymmetric unit accompanied by disordered solvent molecules. The UV-vis spectra of the studied compounds were isomerism and solvent independent, yielding absorption maxima in the vicinity of 400 nm. Their photoluminescence spectra, in turn, strongly depended on isomerism and the used solvent showing smaller Stokes shifts for the emission bands registered in toluene as compared to the corresponding bands measured in dichloromethane. The photoluminescence quantum yields ( $\phi$ ) were systematically higher for toluene solutions reaching the highest value of 20% for p-A. For all three isomers studied, stationary and time-resolved spectroscopic investigations carried out in toluene at different temperatures revealed spectral features indicating a contribution of thermally activated delayed fluorescence (TADF) to the observed spectroscopic behaviour. The measured photoluminescence quantum yields ( $\phi$ ) were higher for solid state films of pure compounds and for their dispersions in solid matrices (zeonex) than those recorded for toluene and dichloromethane solutions of the studied phenoxazine-N-hexylacridone isomers. The obtained experimental spectroscopic and structural data were confronted with theoretical predictions based on DFT calculations.

**Accession Number:** WOS:000537175100024**PubMed ID:** 32301447**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Toman, Petr	B-1834-2009	
Gunka, Piotr A.	D-1295-2012	0000-0002-0977-5246
Wiosna-Salyga, Gabriela	M-3702-2018	0000-0002-4658-7922
Pron, Adam		0000-0002-8267-4353
Banasiewicz, Marzena		0000-0002-8251-5440
Toman, Petr		0000-0002-1607-0332

ISSN: 1463-9076

eISSN: 1463-9084

**Record 40 of 236****Title:** Robust Aluminum and Iron Phosphinate Metal-Organic Frameworks for Efficient Removal of Bisphenol A**Author(s):** Buzek, D (Buzek, Daniel); Ondrusova, S (Ondrusova, Sonja); Hynek, J (Hynek, Jan); Kovar, P (Kovar, Petr); Lang, K (Lang, Kamil); Rohlicek, J (Rohlicek, Jan); Demel, J (Demel, Jan)**Source:** INORGANIC CHEMISTRY Volume: 59 Issue: 8 Pages: 5538-5545 DOI: 10.1021/acs.inorgchem.0c00201 Published: APR 20 2020

**Abstract:** Porous metal-organic frameworks (MOFs) have excellent characteristics for the adsorptive removal of environmental pollutants. Herein, we introduce a new series of highly stable MOFs constructed using Fe<sup>3+</sup> and Al<sup>3+</sup> metal ions and bisphosphinate linkers. The isorecticular design leads to ICR-2, ICR-6, and ICR-7 MOFs with a honeycomb arrangement of linear pores, surface areas up to 1360 m<sup>2</sup> g<sup>-1</sup>, and high solvothermal stabilities. In most cases, their sorption capacity is retained even after 24 h of reflux in water. The choice of the linkers allows for fine-tuning of the pore sizes and the chemical nature of the pores. This feature can be utilized for the optimization of host-guest interactions between molecules and the pore walls. Water pollution by various endocrine disrupting chemicals has been considered a global threat to public health. In this work, we prove that the chemical stability and hydrophobic nature of the synthesized series of MOFs result in the remarkable sorption properties of these materials for endocrine disruptor bisphenol A.

**Accession Number:** WOS:000526885800035**PubMed ID:** 32275140**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lang, Kamil	D-3050-2014	0000-0002-4151-8805
Buzek, Daniel	AAS-3999-2020	
Rohlicek, Jan		0000-0001-6913-2667
Demel, Jan	F-5970-2014	0000-0001-7796-6338

ISSN: 0020-1669

eISSN: 1520-510X

**Record 41 of 236****Title:** The most abundant maternal lncRNA Sirena1 acts post-transcriptionally and impacts mitochondrial distribution**Author(s):** Ganesh, S (Ganesh, Sravya); Horvat, F (Horvat, Filip); Drutovic, D (Drutovic, David); Efenberkova, M (Efenberkova, Michaela); Pinkas, D (Pinkas, Dominik); Jindrova, A (Jindrova, Anna); Pasulka, J (Pasulka, Josef); Iyyappan, R (Iyyappan, Rajan); Malik, R (Malik, Radek); Susor, A (Susor, Andrej); Vlahovick, K (Vlahovick, Kristian); Solc, P (Solc, Petr); Svoboda, P (Svoboda, Petr)**Source:** NUCLEIC ACIDS RESEARCH Volume: 48 Issue: 6 Pages: 3211-3227 DOI: 10.1093/nar/gkz1239 Published: APR 6 2020

**Abstract:** Tens of thousands of rapidly evolving long non-coding RNA (lncRNA) genes have been identified, but functions were assigned to relatively few of them. The lncRNA contribution to the mouse oocyte physiology remains unknown. We report the evolutionary history and functional analysis of Sirena1, the most expressed lncRNA and the 10th most abundant poly(A) transcript in mouse oocytes. Sirena1 appeared in the common ancestor of mouse and rat and became engaged in two different post-transcriptional regulations. First, antisense oriented Bob pseudogene insertion into Sirena1 exon 1 is a source of small RNAs targeting Sob mRNA via RNA interference. Second, Sirena1 evolved functional cytoplasmic polyadenylation elements, an unexpected feature borrowed from translation control of specific maternal mRNAs. Sirena1 knock-out does not affect fertility, but causes minor dysregulation of the maternal transcriptome. This includes increased levels of Elob and mitochondrial mRNAs. Mitochondria in Sirena1(-/-) oocytes disperse from the perinuclear compartment, but do not change in number or ultrastructure. Taken together, Sirena1 contributes to RNA interference and mitochondrial aggregation in mouse oocytes. Sirena1 exemplifies how lncRNAs stochastically engage or even repurpose molecular mechanisms during evolution. Simultaneously, Sirena1 expression levels and unique functional features contrast with the lack of functional importance assessed under laboratory conditions.

**Accession Number:** WOS:000525957500035**PubMed ID:** 31956907**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Iyyappan, Rajan	ABG-7874-2020	0000-0002-6356-7093
Svoboda, Petr	G-3890-2012	0000-0002-4370-3705
Malik, Radek	G-3578-2014	0000-0002-6783-1146

Efenberkova, Michaela	AAF-9968-2020	0000-0003-1227-0393
Solc, Petr	G-7154-2014	0000-0003-4571-3891
Horvat, Filip	S-1904-2017	0000-0002-1896-7645
Jindrova, Anna	E-3968-2018	0000-0003-4334-3268

ISSN: 0305-1048

eISSN: 1362-4962

**Record 42 of 236****Title:** Femtosecond-to-nanosecond dynamics of flavin mononucleotide monitored by stimulated Raman spectroscopy and simulations**Author(s):** Andrikopoulos, PC (Andrikopoulos, Prokopis C.); Liu, YL (Liu, Yingliang); Picchiotti, A (Picchiotti, Alessandra); Lenngren, N (Lenngren, Nils); Kloz, M (Kloz, Miroslav); Chaudhari, AS (Chaudhari, Aditya S.); Precek, M (Precek, Martin); Rebarz, M (Rebarz, Mateusz); Andreasson, J (Andreasson, Jakob); Hajdu, J (Hajdu, Janos); Schneider, B (Schneider, Bohdan); Fuertes, G (Fuertes, Gustavo)**Source:** PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 22 **Issue:** 12 **Pages:** 6538-6552 **DOI:** 10.1039/c9cp04918e **Published:** MAR 28 2020**Abstract:** Flavine mononucleotide (FMN) belongs to the large family of flavins, ubiquitous yellow-coloured biological chromophores that contain an isoalloxazine ring system. As a cofactor in flavoproteins, it is found in various enzymes and photosensory receptors, like those featuring the light-oxygen-voltage (LOV) domain. The photocycle of FMN is triggered by blue light and proceeds via a cascade of intermediate states. In this work, we have studied isolated FMN in an aqueous solution in order to elucidate the intrinsic electronic and vibrational changes of the chromophore upon excitation. The ultrafast transitions of excited FMN were monitored through the joint use of femtosecond stimulated Raman spectroscopy (FSRS) and transient absorption spectroscopy encompassing a time window between 0 ps and 6 ns with 50 fs time resolution. Global analysis of the obtained transient visible absorption and transient Raman spectra in combination with extensive quantum chemistry calculations identified unambiguously the singlet and triplet FMN populations and addressed solvent dynamics effects. The good agreement between the experimental and theoretical spectra facilitated the assignment of electronic transitions and vibrations. Our results represent the first steps towards more complex experiments aimed at tracking structural changes of FMN embedded in light-inducible proteins upon photoexcitation.**Accession Number:** WOS:000526715200027**PubMed ID:** 31994556**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Vives, Gustavo Fuertes	S-8618-2016	0000-0002-8564-8644
liu, Yingliang	AAL-1322-2020	0000-0002-4089-688X
Rebarz, Mateusz	F-7739-2015	0000-0002-5823-2432
Chaudhari, Aditya	AAO-4824-2020	0000-0003-3538-7471
Lenngren, Nils	ABA-3605-2020	
Precek, Martin	G-5648-2014	0000-0002-5790-5543
Andreasson, Jakob		0000-0002-3202-2330
Lenngren, Nils		0000-0001-7563-9843
Schneider, Bohdan	D-2565-2009	0000-0001-7855-3690
Andrikopoulos, Prokopis		0000-0003-0255-1108

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**Record 43 of 236****Title:** Molecular dynamics study of racemic mixtures. II. Temperature dependence of the separation of ibuprofen racemic mixture with beta-cyclodextrin in methanol solvent**Author(s):** Skvara, J (Skvara, Jiri); Nezbeda, I (Nezbeda, Ivo); Izak, P (Izak, Pavel)**Source:** JOURNAL OF MOLECULAR LIQUIDS **Volume:** 302 **Article Number:** 112575 **DOI:** 10.1016/j.molliq.2020.112575 **Published:** MAR 15 2020**Abstract:** Using a realistic united atom interaction model, molecular dynamics simulations were carried out to investigate properties of mixtures of ibuprofen and beta-cyclodextrin both in vacuo and in solution with methanol solvent. The property in focus here is the temperature dependence of the intermolecular interaction energy and the distribution of hydrogen bonds in inclusion complexes established by both the (R)- and (S)-forms of ibuprofen with beta-cyclodextrin. Temperatures were considered in the range from 260 K to 380 K with an increment of 10 K. It was found that (R)-ibuprofen is strongly bonded inside the cyclodextrin molecule, which is more pronounced in the case when the so-called DOWN complex is formed. However, this effect is diminished in the presence of methanol because methanol molecules tend to occupy the majority of possible hydrogen bonding sites. The temperature dependence is not monotonic, and for the DOWN complex in methanol it exhibits two maxima, at 260 K and 310 K. For the UP complex no significant difference was observed at any temperature within the considered range. These results may help both experimentalists and theorists to understand the process of chiral selection of ibuprofen enantiomers. (C) 2020 Elsevier B.V. All rights reserved.**Accession Number:** WOS:000518870300083**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Skvara, Jiri	AAD-3629-2020	

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eISSN: 1873-3166

**Record 44 of 236****Title:** The study of conformational changes in photosystem II during a charge separation**Author(s):** Kulik, N (Kulik, Natalia); Kutý, M (Kutý, Michal); Reha, D (Reha, David)**Source:** JOURNAL OF MOLECULAR MODELING **Volume:** 26 **Issue:** 4 **Article Number:** 75 **DOI:** 10.1007/s00894-020-4332-9 **Published:** MAR 9 2020**Abstract:** Photosystem II (PSII) is a multi-subunit pigment-protein complex and is one of several protein assemblies that function cooperatively in photosynthesis in plants and cyanobacteria. As more structural data on PSII become available, new questions arise concerning the nature of the charge separation in PSII reaction center (RC). The crystal structure of PSII RC from cyanobacteria *Thermosynechococcus vulcanus* was selected for the computational study of conformational changes in photosystem II associated to the charge separation process. The parameterization of cofactors and lipids for classical MD simulation with Amber force field was performed. The parametrized complex of PSII was embedded in the lipid membrane for MD simulation with Amber in Gromacs. The conformational behavior of protein and the cofactors directly involved in the charge separation were studied by MD simulations and QM/MM calculations. This study identified the most likely mechanism of the proton-coupled reduction of plastoquinone Q(B). After the charge separation and the first electron transfer to Q(B), the system undergoes conformational change allowing the first proton transfer to Q(B)(-) mediated via Ser264. After the second electron transfer to Q(B)H, the system again adopts conformation allowing the second proton transfer to Q(B)H(-). The reduced Q(B)H(2) would then leave the binding pocket.**Accession Number:** WOS:000519593600001**PubMed ID:** 32152736**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kutý, Michal	D-9309-2016	0000-0002-6149-3123
Kulik, Natalia	H-4497-2014	
Reha, David		0000-0002-9500-0569

ISSN: 1610-2940

eISSN: 0948-5023

**Record 45 of 236****Title:** Cascade disruptions in asteroid clusters**Author(s):** Fatka, P (Fatka, Petr); Pravec, P (Pravec, Petr); Vokrouhlický, D (Vokrouhlický, David)**Source:** ICARUS **Volume:** 338 **Article Number:** 113554 **DOI:** 10.1016/j.icarus.2019.113554 **Published:** MAR 1 2020**Abstract:** We studied asteroid clusters suggesting a possibility of at least two disruption events in their recent history ( $\leq 5$  Myr). We searched for new members of known asteroid pairs and clusters and we verified their membership using backward orbital integrations. We found four asteroid clusters, namely the clusters of (11842) Kap'bos, (14627) Emilkowalski, (63440) 2001 MD30 and (157123) 2004 NW5 that show at least two secondary separation events that occurred at significantly different times. We considered a possible formation mechanism for these clusters: The parent of an asteroid cluster was spun up to its critical rotation frequency, underwent a rotation fission and was slowed down by escape of the newly formed secondary/ies. Then the YORP effect spun up the primary again and it reached its critical rotation frequency and underwent another fission. We created a simple model

to test whether the scenario of two rotation fission events of a parent primary induced via the YORP effect is possible for the four clusters. We obtained a good agreement between the model and the cluster properties for the clusters of Kap'bos and (63440). For the cluster of Emilkowalski, our model explained the unusually slow rotation of the primary. However, the time needed for the primary to reach its critical frequency after the first fission event was predicted to be too long by a factor of several. We suspect, considering also its D type taxonomic classification and the existence of a dust band associated with the cluster, that the asteroid Emilkowalski may actually be a cometary nucleus. Regarding the cluster of (157123), the final rotational frequency of the primary after the last fission event predicted by our model is in a good agreement with the observed rotation frequency of (157123). However, a separation of the older secondary is not possible in our model due to the deficiency of free energy needed for an escape of the large secondary. This could be due to an error in the H value of the secondary or the possibility that we did not find the real primary of this cluster.

**Accession Number:** WOS:000516888000037

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Fatka, Petr	ABA-9140-2020	0000-0003-1127-9302
Pravec, Petr	AAE-2695-2019	0000-0001-8434-9776

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#### Record 46 of 236

**Title:** Isoforms of Cathepsin B1 in Neurotropic Schistosomula of *Trichobilharzia regenti* Differ in Substrate Preferences and a Highly Expressed Catalytically Inactive Paralog Binds Cystatin

**Author(s):** Dvorakova, H (Dvorakova, Hana); Leontovyc, R (Leontovyc, Roman); Machacek, T (Machacek, Tomas); O'Donoghue, AJ (O'Donoghue, Anthony J.); Sedo, O (Sedo, Ondrej); Zdrahal, Z (Zdrahal, Zbynek); Craik, CS (Craik, Charles S.); Caffrey, CR (Caffrey, Conor R.); Horak, P (Horak, Petr); Mikes, L (Mikes, Libor)

**Source:** FRONTIERS IN CELLULAR AND INFECTION MICROBIOLOGY **Volume:** 10 **Article Number:** 66 **DOI:** 10.3389/fcimb.2020.00066 **Published:** FEB 26 2020

**Abstract:** Schistosomula (the post-infective stages) of the neurotropic schistosome *Trichobilharzia regenti* possess multiple isoforms of cathepsin B1 peptidase (TrCB1.1-TrCB1.6) with involvement in nutrient digestion. The comparison of substrate preferences of TrCB1.1 and TrCB1.4 showed that TrCB1.4 had a very narrow substrate specificity and after processing it was less effective toward protein substrates when compared to TrCB1.1. Self-processing of both isoforms could be facilitated by sulfated polysaccharides due to a specific binding motif in the pro-sequence. Trans-activation by heterologous enzymes was also successfully employed. Expression profiling revealed a high level of transcription of genes encoding the enzymatically inactive paralogs TrCB1.5 and TrCB1.6. The transcription level of TrCB1.6 was comparable with that of TrCB1.1 and TrCB1.2, the most abundant active isoforms.

Recombinant TrCB1.6wt, a wild type paralog with a Cys(29)-to-Gly substitution in the active site that renders the enzyme inactive, was processed by the active TrCB1 forms and by an asparaginyl endopeptidase. Although TrCB1.6wt lacked hydrolytic activity, endopeptidase, but not dipeptidase, activity could be restored by mutating Gly(29) to Cys(29). The lack of exopeptidase activity may be due to other mutations, such as His(110)-to-Asn in the occluding loop and Asp(224)-to-Gly in the main body of the mature TrCB1.6, which do not occur in the active isoforms TrCB1.1 and TrCB1.4 with exopeptidase activity. The catalytically active enzymes and the inactive TrCB1.6 paralog formed complexes with chicken cystatin, thus supporting experimentally the hypothesis that inactive paralogs could potentially regulate the activity of the active forms or protect them from being inhibited by host inhibitors. The effect on cell viability and nitric oxide production by selected immune cells observed for TrCB1.1 was not confirmed for TrCB1.6. We show here that the active isoforms of TrCB1 have different affinities for peptide substrates thereby facilitating diversity in protein-derived nutrition for the parasite. The inactive paralogs are unexpectedly highly expressed and one of them retains the ability to bind cystatins, likely due to specific mutations in the occluding loop and the enzyme body. This suggests a role in sequestration of inhibitors and protection of active cysteine peptidases.

**Accession Number:** WOS:000524706100001

**PubMed ID:** 32175287

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Machacek, Tomas	B-6274-2016	0000-0002-6310-4099
Horak, Petr	C-6482-2009	0000-0001-9820-5044
Mikes, Libor	J-8551-2017	0000-0002-2440-6641
Zdrahal, Zbynek		0000-0003-3044-5548

ISSN: 2235-2988

#### Record 47 of 236

**Title:** Eu@C-86 isomers: Calculated relative populations

**Author(s):** Slanina, Z (Slanina, Zdenek); Uhlik, F (Uhlik, Filip); Bao, LP (Bao, Lipiao); Akasaka, T (Akasaka, Takeshi); Lu, X (Lu, Xing); Adamowicz, L (Adamowicz, Ludwik)

**Source:** FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES **Volume:** 28 **Issue:** 7 **Pages:** 565-570 **DOI:** 10.1080/1536383X.2020.1724104 **Early Access Date:** FEB 2020 **Published:** JUL 2 2020

**Abstract:** Relative populations of four energy-lowest IPR (isolated-pentagon-rule) isomers of Eu@C-86 are computed using the Gibbs energy based on characteristic from density functional theory calculations (M06-2X/3-21G similar to SDD entropy term, M06-2X/6-31G\* similar to SDD or B2PLYP(D)/6-31G\* similar to SDD energetics). The calculations confirm that the recently isolated Eu@C-1(7)-C-86 species is a major isomer in a relevant temperature region. Relationship to the empty C-86 cages is discussed, too.

**Accession Number:** WOS:000513597800001

ISSN: 1536-383X

eISSN: 1536-4046

#### Record 48 of 236

**Title:** Multi-phase ELAStic Aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites

**Author(s):** Friak, M (Friak, M.); Lago, D (Lago, D.); Koutna, N (Koutna, N.); Holec, D (Holec, D.); Rebok, T (Rebok, T.); Sob, M (Sob, M.)

**Source:** COMPUTER PHYSICS COMMUNICATIONS **Volume:** 247 **Article Number:** 106863 **DOI:** 10.1016/j.cpc.2019.106863 **Published:** FEB 2020

**Abstract:** We introduce a new web-based tool called MELASA (Multi-phase ELAStic Aggregates), open-access available at <https://melasa.cerit-sc.cz>, for computations and visualizations of anisotropic elastic properties of lamellar (nano-)composites. MELASA implements a linear-elasticity method by Grimsditch and Nizzoli (1986), originally developed for superlattices of any symmetry. Our tool may be used for computation of anisotropic elastic properties of a specific type of periodically separated lamellar (nano-) composites using matrices of elastic stiffnesses of co-existing phases as an input. Elastic properties are visualized in the form of directional dependencies of selected elastic characteristics (Young's modulus and linear compressibility). MELASA further generalizes the Grimsditch-Nizzoli approach, which was originally formulated for only two phases, to multiple-phase composites. Additionally, our implementation allows for treating internal rotations of local coordination systems corresponding to the natural set of coordinates that match directional vectors of unit cell defining crystal lattice within the co-existing phases. Fe-Al-based superalloy nanocomposites are employed as a numerical example of superlattices with the input and output elastic stiffnesses determined by quantum-mechanical calculations. In particular, three different atomic configurations of interfaces in superlattices containing the ordered Fe-Al phase and a disordered Fe-Al phase with 18.75at.%Al (modeled by a special quasi-random structure, SQS) are considered. They differ by relative positions of sublattices in Fe-Al (an antiphase-like shift) and/or atomic planes in Fe-18.75at.%Al with respect to the interface (a circular/cyclic shift).

Program summary

Program title: MELASA

Program files doi: <http://dx.doi.org/10.17632/rzc2yd2rvc.1>

Licensing provisions: MIT license

Programming language: JavaScript

Nature of problem: Computations and visualizations of anisotropic elastic properties of lamellar (nano-)composites/superlattices

Solution method: Implementation of a linear-elasticity method by M. Grimsditch and F. Nizzoli 111, originally derived for superlattices of any symmetry. MELASA computes anisotropic elastic properties of a specific type of periodically separated lamellar (nano-)composites using matrices of elastic stiffnesses of co-existing phases as input. Elastic properties are visualized in the form of directional dependencies of selected elastic characteristics (Young's modulus and linear compressibility).

Additional comments including restrictions and unusual features: MELASA generalizes the GrimsditchNizzoli approach, which was originally formulated for only two phases, to multiple-phase composites. Additionally, our implementation allows for treating internal rotations of local coordination systems corresponding to the natural set of coordinates that match directional vectors of unit cell defining crystal lattice within the co-existing phases. (C) 2019 Elsevier B.V. All rights reserved.

**Accession Number:** WOS:000503093400014

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
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Holec, David	AAB-8738-2020	0000-0002-3516-1061
Sob, Mojmir	G-6865-2011	0000-0002-5724-890X
Koutna, Nikola		0000-0001-7901-4736

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**Record 49 of 236****Title:** Sparse sampling and tensor network representation of two-particle Green's functions**Author(s):** Shinaoka, H (Shinaoka, Hiroshi); Geffroy, D (Geffroy, Dominique); Wallerberger, M (Wallerberger, Markus); Otsuki, J (Otsuki, Junya); Yoshimi, K (Yoshimi, Kazuyoshi); Gull, E (Gull, Emanuel); Kunes, J (Kunes, Jan)**Source:** SCIPost PHYSICS **Volume:** 8 **Issue:** 1 **Article Number:** 012 **DOI:** 10.21468/SciPostPhys.8.1.012 **Published:** JAN 2020**Abstract:** Many-body calculations at the two-particle level require a compact representation of two-particle Green's functions. In this paper, we introduce a sparse sampling scheme in the Matsubara frequency domain as well as a tensor network representation for two-particle Green's functions. The sparse sampling is based on the intermediate representation basis and allows an accurate extraction of the generalized susceptibility from a reduced set of Matsubara frequencies. The tensor network representation provides a system independent way to compress the information carried by two-particle Green's functions. We demonstrate efficiency of the present scheme for calculations of static and dynamic susceptibilities in single- and two-band Hubbard models in the framework of dynamical mean-field theory.**Accession Number:** WOS:000512377100012**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kunes, Jan	B-4484-2008	0000-0001-9682-7640
Shinaoka, Hiroshi	L-9288-2018	0000-0002-7058-8765
Gull, Emanuel	A-2362-2010	0000-0002-6082-1260
Geffroy, Dominique	J-3887-2013	0000-0003-2785-2679

ISSN: 2542-4653

**Record 50 of 236****Title:** Linear transformations for cross-lingual semantic textual similarity**Author(s):** Brychcin, T (Brychcin, Tomas)**Source:** KNOWLEDGE-BASED SYSTEMS **Volume:** 187 **Article Number:** 104819 **DOI:** 10.1016/j.knosys.2019.06.027 **Published:** JAN 2020**Abstract:** Cross-lingual semantic textual similarity systems estimate the degree of the meaning similarity between two sentences, each in a different language. State-of-the-art algorithms usually employ machine translation and combine vast amount of features, making the approach strongly supervised, resource rich, and difficult to use for poorly-resourced languages.

In this paper, we study linear transformations, which project monolingual semantic spaces into a shared space using bilingual dictionaries. We propose a novel transformation, which builds on the best ideas from prior works. We experiment with unsupervised techniques for sentence similarity based only on semantic spaces and we show they can be significantly improved by the word weighting. Our transformation outperforms other methods and together with word weighting leads to very promising results on several datasets in different languages. (C) 2019 Elsevier B.V. All rights reserved.

**Accession Number:** WOS:000501653900008**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Brychcin, Tomas	C-1181-2016	0000-0002-7442-0978

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## Record 51 of 236

**Title:** Nonequilibrium steady-state picture of incoherent light-induced excitation harvesting**Author(s):** Jankovic, V (Jankovic, Veljko); Mancal, T (Mancal, Tomas)**Source:** JOURNAL OF CHEMICAL PHYSICS **Volume:** 153 **Issue:** 24 **Article Number:** 244110 **DOI:** 10.1063/5.0029918 **Published:** DEC 28 2020**Abstract:** We formulate a comprehensive theoretical description of excitation harvesting in molecular aggregates photoexcited by weak incoherent radiation. An efficient numerical scheme that respects the continuity equation for excitation fluxes is developed to compute the nonequilibrium steady state (NESS) arising from the interplay between excitation generation, excitation relaxation, dephasing, trapping at the load, and recombination. The NESS is most conveniently described in the so-called preferred basis in which the steady-state excitonic density matrix is diagonal. The NESS properties are examined by relating the preferred-basis description to the descriptions in the site or excitonic bases. Focusing on a model photosynthetic dimer, we find that the NESS in the limit of long trapping time is quite similar to the excited-state equilibrium in which the stationary coherences originate from the excitation-environment entanglement. For shorter trapping times, we demonstrate how the properties of the NESS can be extracted from the time-dependent description of an incoherently driven but unloaded dimer. This relation between stationary and time-dependent pictures is valid, provided that the trapping time is longer than the decay time of dynamic coherences accessible in femtosecond spectroscopy experiments.**Accession Number:** WOS:000603068300010**PubMed ID:** 33380098**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Jankovic, Veljko	L-2169-2019	0000-0002-0297-2167
Jankovic, Veljko	C-3485-2019	0000-0002-0297-2167

ISSN: 0021-9606

eISSN: 1089-7690

## Record 52 of 236

**Title:** The wide-spectrum antimicrobial effect of novel N-alkyl monoquaternary ammonium salts and their mixtures; the QSAR study against bacteria**Author(s):** Soukup, O (Soukup, Ondrej); Benkova, M (Benkova, Marketa); Dolezal, R (Dolezal, Rafael); Sleha, R (Sleha, Radek); Malinak, D (Malinak, David); Salajkova, S (Salajkova, Sarka); Markova, A (Markova, Aneta); Hympanova, M (Hympanova, Michaela); Prchal, L (Prchal, Lukas); Ryskova, L (Ryskova, Lenka); Hobzova, L (Hobzova, Lenka); Sepcic, K (Sepcic, Kristina); Gunde-Cimerman, N (Gunde-Cimerman, Nina); Korabecny, J (Korabecny, Jan); Jun, D (Jun, Daniel); Bostikova, V (Bostikova, Vanda); Bostik, P (Bostik, Pavel); Marek, J (Marek, Jan)**Source:** EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY **Volume:** 206 **Article Number:** 112584 **DOI:** 10.1016/j.ejmech.2020.112584 **Published:** NOV 15 2020**Abstract:** Quaternary ammonium salts (QASs) have been widely used for disinfection purposes because of their low price, high efficacy and low human toxicity for decades. However, precise mechanisms of action nor the powerful versatile agent against all antimicrobial species are known. In this study we have prepared 43 novel N-alkyl monoquaternary ammonium salts including 7 N,N-dialkyl monoquaternary ammonium salts differing bearing alkyl chain either of 12, 14 or 16 carbons. Together with 15 already published QASs we have studied the antimicrobial efficacy of all water-soluble compounds together with standard benzalkonium salts against Gram-positive (G+) and Gram-negative (G-) bacteria, anaerobic spore-forming *Cl. difficile*, yeasts, filamentous fungi and enveloped Varicella zoster virus (VZV). To address the mechanism of action, lipophilicity seems to be a key parameter which determines antimicrobial efficacy, however, exceptions are likely to occur and therefore QSAR analysis on the efficacy against G+ and G- bacteria was applied. We showed that antibacterial activity is higher when the molecule is larger, more lipophilic, less polar, and contains fewer oxygen atoms, fewer methyl groups bound to heteroatoms or fewer hydrogen atoms bound to polarized carbon atoms. In addition, from an application point of view, we have formulated mixtures, on the basis of obtained efficiency of individual compounds, in order to receive wide-spectrum agent. All formulated mixtures completely eradicated tested G+ and G- strains, including the multidrug-resistant *P. aeruginosa* as well as in case of yeasts. However, effect on *A. fumigatus*, *Cl. difficile* and VZV the exposition towards mixture resulted in significant reduction only. Finally, 3 out of 4 formulated mixtures were safer than reference commercial agent based on benzal-konium salts only in the skin irritation test using reconstructed human epidermidis. (C) 2020 Elsevier Masson SAS. All rights reserved.**Accession Number:** WOS:000579097000004**PubMed ID:** 32853858**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Malinak, David	AAH-1337-2020	
Malinak, David		0000-0002-0665-0667
Korabecny, Jan	J-6362-2018	0000-0001-6977-7596

ISSN: 0223-5234

eISSN: 1768-3254

## Record 53 of 236

**Title:** Efficient adsorption of endocrine-disrupting pesticides from water with a reusable magnetic covalent organic framework**Author(s):** Romero, V (Romero, Vanesa); Fernandes, SPS (Fernandes, Soraia P. S.); Kovar, P (Kovar, Petr); Psenicka, M (Psenicka, Milan); Kolen'ko, YV (Kolen'ko, Yury, V); Salonen, LM (Salonen, Laura M.); Espina, B (Espina, Begona)**Source:** MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 307 **Article Number:** 110523 **DOI:** 10.1016/j.micromeso.2020.110523 **Published:** NOV 2020**Abstract:** A magnetic covalent organic framework (COF) is applied for the first time as adsorbent for the extraction of endocrine-disrupting pesticides from water. High adsorption efficiencies were found for lipophilic chlorpyrifos and atrazine, with calculated maximum adsorption capacities of 270 mg g<sup>-1</sup> and 54 mg g<sup>-1</sup>, respectively, outperforming reported adsorbents, such as activated carbon, graphene, or metal-organic frameworks. Polar diquat showed very poor adsorption efficiency, indicating that hydrophobic interactions play a role in the adsorption. Calculations revealed that the interactions between the COF and the pesticides are mainly based on van der Waals interactions. Finally, recycling experiments showed that both pesticides can be recovered with an efficiency of over 90% using acetonitrile as solvent, with merely minor losses in adsorption capacity after five consecutive cycles of adsorption/desorption. The present study promotes further exploration of the possible application of COFs for the extraction and pre-concentration of pesticides in environmental matrices.**Accession Number:** WOS:000572431000008**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Espina, Begona	ABG-2611-2020	0000-0002-7645-2834
Kolen'ko, Yury	P-5890-2015	0000-0001-7493-1762
Romero, Vanesa		0000-0003-3528-3576
Salonen, Laura	I-3920-2016	0000-0001-8194-6014

ISSN: 1387-1811

eISSN: 1873-3093

## Record 54 of 236

**Title:** Selective inhibition of aldo-keto reductase 1C3: a novel mechanism involved in midostaurin and daunorubicin synergism**Author(s):** Morell, A (Morell, Anselm); Novotna, E (Novotna, Eva); Milan, J (Milan, Jaroslav); Danielisova, P (Danielisova, Petra); Bukum, N (Bukum, Neslihan); Wsol, V (Wsol, Vladimir)**Source:** ARCHIVES OF TOXICOLOGY **Volume:** 95 **Issue:** 1 **Pages:** 67-78 **DOI:** 10.1007/s00204-020-02884-2 **Early Access Date:** OCT 2020 **Published:** JAN 2021**Abstract:** Midostaurin is an FMS-like tyrosine kinase 3 receptor (FLT3) inhibitor that provides renewed hope for treating acute myeloid leukaemia (AML). The limited efficacy of this compound as a monotherapy contrasts with that of its synergistic combination with standard cytarabine and daunorubicin (Dau), suggesting a therapeutic benefit that is not driven only by FLT3 inhibition. In an AML context, the activity of the enzyme aldo-keto reductase 1C3 (AKR1C3) is a crucial factor in chemotherapy resistance, as it mediates the intracellular transformation of anthracyclines to less active hydroxy metabolites. Here, we report that midostaurin is a potent inhibitor of Dau inactivation mediated by AKR1C3 in both its recombinant form as well as during its overexpression in a transfected cell model. Likewise, in the FLT3(-)JAML cell line KG1a, midostaurin was able to increase the cellular accumulation of Dau and significantly decrease its metabolism by AKR1C3 simultaneously. The combination of those mechanisms increased the nuclear localization of Dau, thus synergizing its cytotoxic effects on KG1a cells. Our results provide new in vitro evidence of how the therapeutic activity of midostaurin could operate beyond targeting the FLT3

receptor.

**Accession Number:** WOS:000575709900002**PubMed ID:** 33025066**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Wsol, Vladimir	K-3476-2016	0000-0003-3745-7648
Morell, Anselm		0000-0001-7002-7792

**ISSN:** 0340-5761**eISSN:** 1432-0738**Record 55 of 236****Title:** Origin of the Unusual Stability of Zeolite-Encapsulated Sub-Nanometer Platinum**Author(s):** Hou, DW (Hou, Dianwei); Grajciar, L (Grajciar, Lukas); Nachtigall, P (Nachtigall, Petr); Heard, CJ (Heard, Christopher J.)**Source:** ACS CATALYSIS Volume: 10 Issue: 19 Pages: 11057-11068 DOI: 10.1021/acscatal.0c01344 Published: OCT 2 2020

**Abstract:** The mechanism by which single metal atoms and small, zeolite-encapsulated metal particles are stabilized against migration and growth is not currently well understood. In this work, we employ an unbiased density functional global optimization strategy to identify the locations and energetic barriers for migration pathways between sites for platinum (Pt) confined within the microporous volume of a purely silicious zeolite with Linde type A topology and its aluminosilicate and borosilicate variants. We observe an impressive stabilization of single Pt atoms caused by a hitherto unreported binding mode, in which the six rings in the framework are broken, leading to trapped, highly accessible metal centers. In addition, heteroatom substituents are found to significantly enhance the incorporation of Pt via an unexpected insertion into framework SiO-H bonds. Migration of Pt is hindered by high barriers, which are predicted to vary significantly with Si:X (X = Al and B) ratios. It is proposed that an optimal Si:X ratio exists for a given zeolite topology, in which the barriers will reach the maximum value. The energetic preference for Pt clustering (via Ostwald ripening) remains but is significantly reduced with respect to isolated clusters because of the strong interactions between Pt atoms and the framework. Our findings suggest a means to control noble-metal particle sintering, despite a thermodynamic driving force toward Pt clustering. This work provides an explanation for the surprisingly high degree of kinetic stability of ultrasmall, encapsulated metal particles observed experiment.

**Accession Number:** WOS:000577156300020**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Nachtigall, Petr	A-6220-2013	0000-0002-1628-7275
Grajciar, Lukas	H-1266-2015	0000-0001-9464-7769
Heard, Christopher	L-5965-2017	0000-0001-8034-6121
Hou, Dianwei	E-1347-2017	0000-0002-5077-291X

**ISSN:** 2155-5435**Record 56 of 236****Title:** Activation of glycogenolysis and glycolysis in breast cancer stem cell models**Author(s):** Abad, E (Abad, Etna); Samino, S (Samino, Sara); Yanes, O (Yanes, Oscar); Potesil, D (Potesil, David); Zdrahal, Z (Zdrahal, Zbynek); Lyakhovich, A (Lyakhovich, Alex)**Source:** BIOCHIMICA ET BIOPHYSICA ACTA-MOLECULAR BASIS OF DISEASE Volume: 1866 Issue: 10 Article Number: 165886 DOI: 10.1016/j.bbadis.2020.165886 Published: OCT 1 2020**Accession Number:** WOS:000559983700004**PubMed ID:** 32592934**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lyakhovich, Alex	B-4410-2008	0000-0002-8279-4697

**ISSN:** 0925-4439**eISSN:** 1879-260X**Record 57 of 236****Title:** Electronic continuum correction without scaled charges**Author(s):** Predota, M (Predota, Milan); Biriukov, D (Biriukov, Denys)**Source:** JOURNAL OF MOLECULAR LIQUIDS Volume: 314 Article Number: 113571 DOI: 10.1016/j.molliq.2020.113571 Published: SEP 15 2020

**Abstract:** In recent years the "Pandora's box" of charges used in classical simulations of nonpolarizable molecular models, especially for aqueous solutions and ionic liquids, has been opened. Particularly we refer to the Electronic continuum correction (ECC) model that suggests applying scaled down charges of ions and tearing down the 'dogma' of identical charges used to describe the potential energy surfaces (PES) and dipole moment surface (DMS). We elaborate on both ideas and integrate them into a consistent description of 'real' atomic charges of water and ions, which does not necessarily need to violate the 'dogma'. We promote ECC epsilon approach directly incorporating the electronic polarizability into screening of electrostatic interactions, avoiding the use of scaled charges, which perplex the comparison with experiment, ab initio or polarizable models and are cumbersome for interactions with external electric or magnetic fields. We conclude that none of the existing nonpolarizable water models is fully consistent with the continuum electronic polarizability and stimulate a quest for a better model implementing ECC epsilon ideas. (C) 2020 Elsevier B.V. All rights reserved.

**Accession Number:** WOS:000561905700015**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Biriukov, Denys	Q-4898-2018	0000-0003-1007-2203
Predota, Milan	A-2256-2009	0000-0003-3902-0992

**ISSN:** 0167-7322**eISSN:** 1873-3166**Record 58 of 236****Title:** Binary asteroid (31) Euphrosyne: ice-rich and nearly spherical

**Author(s):** Yang, B (Yang, B.); Hanus, J (Hanus, J.); Carry, B (Carry, B.); Vernazza, P (Vernazza, P.); Broz, M (Broz, M.); Vachier, F (Vachier, F.); Rambaux, N (Rambaux, N.); Marsset, M (Marsset, M.); Chrenko, O (Chrenko, O.); Sevecek, P (Sevecek, P.); Viikinkoski, M (Viikinkoski, M.); Jehin, E (Jehin, E.); Ferrais, M (Ferrais, M.); Podlowska-Gaca, E (Podlowska-Gaca, E.); Drouard, A (Drouard, A.); Marchis, F (Marchis, F.); Birlan, M (Birlan, M.); Benkhaldoun, Z (Benkhaldoun, Z.); Berthier, J (Berthier, J.); Bartczak, P (Bartczak, P.); Dumas, C (Dumas, C.); Dudzinski, G (Dudzinski, G.); Durech, J (Durech, J.); Castillo-Rogez, J (Castillo-Rogez, J.); Cipriani, F (Cipriani, F.); Colas, F (Colas, F.); Fetick, R (Fetick, R.); Fusco, T (Fusco, T.); Grice, J (Grice, J.); Jorda, L (Jorda, L.); Kaasalainen, M (Kaasalainen, M.); Kryszyzowska, A (Kryszyzowska, A.); Lamy, P (Lamy, P.); Marciniak, A (Marciniak, A.); Michalowski, T (Michalowski, T.); Michel, P (Michel, P.); Pajuelo, M (Pajuelo, M.); Santana-Ros, T (Santana-Ros, T.); Tanga, P (Tanga, P.); Vigan, A (Vigan, A.); Witasse, O (Witasse, O.)

**Source:** ASTRONOMY & ASTROPHYSICS Volume: 641 Article Number: A80 DOI: 10.1051/0004-6361/202038372 Published: SEP 11 2020

**Abstract:** Aims. Asteroid (31) Euphrosyne is one of the biggest objects in the asteroid main belt and it is also the largest member of its namesake family. The Euphrosyne family occupies a highly inclined region in the outer main belt and contains a remarkably large number of members, which is interpreted as an outcome of a disruptive cratering event. Methods. The goals of this adaptive-optics imaging study are threefold: to characterize the shape of Euphrosyne, to constrain its density, and to search for the large craters that may be associated with the family formation event.

Results. We obtained disk-resolved images of Euphrosyne using SPHERE/ZIMPOL at the ESO 8.2 m VLT as part of our large program (ID: 199.C-0074, PI: Vernazza). We reconstructed its 3D shape via the ADAM shape modeling algorithm based on the SPHERE images and the available light curves of this asteroid. We analyzed the dynamics of the satellite with the Genoid meta-heuristic algorithm. Finally, we studied the shape of Euphrosyne using hydrostatic equilibrium models.

Conclusions. Our SPHERE observations show that Euphrosyne has a nearly spherical shape with the sphericity index of 0.9888 and its surface lacks large impact craters. Euphrosyne's diameter is 268 +/- 6 km, making it one of the top ten largest main belt asteroids. We detected a satellite of Euphrosyne - S/2019 (31) 1 - that is about 4 km across, on a circular orbit. The mass determined from the orbit of the satellite together with the volume computed from the shape model imply a density of 1665 +/- 242 kg m<sup>-3</sup>, suggesting that Euphrosyne probably contains a large fraction of water ice in its interior. We find that the spherical shape of Euphrosyne is a result of the reaccumulation process following the impact, as in the case of (10) Hygiea. However, our shape analysis reveals that, contrary to Hygiea, the axis ratios of Euphrosyne significantly differ from those suggested by fluid hydrostatic equilibrium





Author	Web of Science ResearcherID	ORCID Number
Bartolini, Andrea	P-3440-2019	0000-0002-1148-2450
Vysocky, Ondrej		0000-0001-7849-2744

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eISSN: 1532-0634

**Record 63 of 236****Title:** New Fast ApEn and SampEn Entropy Algorithms Implementation and Their Application to Supercomputer Power Consumption**Author(s):** Tomcala, J (Tomcala, Jiri)**Source:** ENTROPY **Volume:** 22 **Issue:** 8 **Article Number:** 863 **DOI:** 10.3390/e22080863 **Published:** AUG 2020

**Abstract:** Approximate Entropy and especially Sample Entropy are recently frequently used algorithms for calculating the measure of complexity of a time series. A lesser known fact is that there are also accelerated modifications of these two algorithms, namely Fast Approximate Entropy and Fast Sample Entropy. All these algorithms are effectively implemented in the R software package TSEntropies. This paper contains not only an explanation of all these algorithms, but also the principle of their acceleration. Furthermore, the paper contains a description of the functions of this software package and their parameters, as well as simple examples of using this software package to calculate these measures of complexity of an artificial time series and the time series of a complex real-world system represented by the course of supercomputer infrastructure power consumption. These time series were also used to test the speed of this package and to compare its speed with another R package pracma. The results show that TSEntropies is up to 100 times faster than pracma and another important result is that the computational times of the new Fast Approximate Entropy and Fast Sample Entropy algorithms are up to 500 times lower than the computational times of their original versions. At the very end of this paper, the possible use of this software package TSEntropies is proposed.

**Accession Number:** WOS:000564074400001**PubMed ID:** 33286634**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Tomcala, Jiri		0000-0002-0940-527X

eISSN: 1099-4300

**Record 64 of 236****Title:** Effect of Helical Kink on Peptide Translocation across Phospholipid Membranes**Author(s):** Brozek, R (Brozek, Radim); Kabelka, I (Kabelka, Ivo); Vacha, R (Vacha, Robert)**Source:** JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 124 **Issue:** 28 **Pages:** 5940-5947 **DOI:** 10.1021/acs.jpcc.0c03291 **Published:** JUL 16 2020

**Abstract:** Biological membranes present a major obstacle for the delivery of therapeutic agents into cells. Some peptides have been shown to translocate across the membrane spontaneously, and they could be thus used as drug-carriers. However, the advantageous peptide properties for the translocation remain unclear. Of particular interest is the effect of a proline-induced kink in  $\alpha$ -helical peptides, because the kink was previously reported to both increase and decrease the antimicrobial activity. The antimicrobial activity of peptides could be related to their translocation across the membrane as is the case of the buforin 2 peptide investigated here. Using computer simulations with two independent models, we consistently showed that the presence of the kink has (1) no effect on the translocation barrier, (2) reduces the peptide affinity to the membrane, and (3) disfavors the transmembrane state. Moreover, we were able to determine that these effects are mainly caused by the peptide increased polarity, not the increased flexibility of the kink. The provided molecular understanding can be utilized for the design of cell-penetrating and drug-carrying peptides.

**Accession Number:** WOS:000551541600017**PubMed ID:** 32603116

ISSN: 1520-6106

eISSN: 1520-5207

**Record 65 of 236****Title:** Passive Optical Networks Progress: A Tutorial**Author(s):** Horvath, T (Horvath, Tomas); Munster, P (Munster, Petr); Ujezsky, V (Ujezsky, Vaclav); Bao, NH (Bao, Ning-Hai)**Source:** ELECTRONICS **Volume:** 9 **Issue:** 7 **Article Number:** 1081 **DOI:** 10.3390/electronics9071081 **Published:** JUL 2020

**Abstract:** For many years, passive optical networks (PONs) have received a considerable amount of attraction regarding their potential for providing broadband connectivity to almost every citizen, especially in remote areas where fiber optics can attract people to populate regions that have been abandoned. Error-free connectivity without dropouts can offer new opportunities to communicate, earn money and enjoy cultural events. Transmission speeds are multigigabit with distances of a few tens of kilometers; these specifications were previously reserved for high-speed and long-haul backbone networks. PONs can also support a new class of applications, such as accurate time transfer or distributed fiber sensing and follow new trends in open networking. An outline of past and current standards and standards that have been proposed for the latest generation of multigigabit PONs is provided.

**Accession Number:** WOS:000558054900001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Ujezsky, Vaclav	Q-9784-2017	0000-0001-7629-6299
Munster, Petr	F-6942-2019	0000-0002-4651-8353

eISSN: 2079-9292

**Record 66 of 236****Title:** Numerical microstructure model of NiTi wire reconstructed from 3D-XRD data**Author(s):** Heller, L (Heller, L.); Karafiatova, I (Karafiatova, I); Petrich, L (Petrich, L.); Pawlas, Z (Pawlas, Z.); Shayanfard, P (Shayanfard, P.); Benes, V (Benes, V); Schmidt, V (Schmidt, V); Sittner, P (Sittner, P.)**Source:** MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING **Volume:** 28 **Issue:** 5 **Article Number:** 055007 **DOI:** 10.1088/1361-651X/ab89c1 **Published:** JUL 2020

**Abstract:** In this paper, the grain microstructure and strain partitioning in a polycrystalline NiTi wire subjected to tensile loading was reconstructed from an experimental 3D-XRD dataset. The reconstruction of a volume containing more than 8000 stressed grains involved optimization with respect to both the geometrical features and material elastic properties. The geometrical features of the microstructure were reconstructed using Laguerre tessellations based on the experimental 3D-XRD dataset. Two different algorithms fitting Laguerre tessellations were applied in order to assess the sensitivity of the reconstruction to the choice of the algorithm. The material properties in terms of elastic anisotropy were refined from an initial published value to minimize the mismatch between experiment and simulation using an optimization algorithm based on linear elasticity simulations. As a result of this, we constructed a numerical microstructure model that statistically matches the experimentally probed material in terms of positions and sizes of grains as well as partitioning of elastic strain and stress in the microstructure (average elastic properties and standard deviations of piecewise constant components of elastic strain and stress tensors in grains).

**Accession Number:** WOS:000536678300001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Benes, Viktor	J-6620-2017	0000-0002-0605-0135
Pawlas, Zbynek	D-1764-2017	0000-0002-1042-8073
Shayanfard, Pejman		0000-0001-7847-0369
Heller, Ludek	B-2770-2011	0000-0002-4901-541X
Karafiatova, Iva		0000-0002-6473-8480

ISSN: 0965-0393

eISSN: 1361-651X

**Record 67 of 236****Title:** Distribution of O atoms on partially oxidized metal targets, and the consequences for reactive sputtering of individual metal oxides**Author(s):** Houska, J (Houska, J.); Kozak, T (Kozak, T.)**Source:** SURFACE & COATINGS TECHNOLOGY **Volume:** 392 **Article Number:** 125685 **DOI:** 10.1016/j.surfcoat.2020.125685 **Published:** JUN 25 2020

**Abstract:** We investigate the oxidation of a wide range of metal surfaces by ab-initio calculations. We go through a wide range of metals (Sc, Y, La, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, W, Cu, Ag, Au, Zn, Cd, Al) and surface oxygen coverages ( $\theta(O)$ ). Calculations of the adsorption energy per O atom ( $E_{\text{ads\_mm}}$ ) are followed by characterizing the preferred distribution of O atoms on a partially oxidized surface (considering up to 329 distributions per metal). We find that individual metals exhibit qualitatively different  $E_{\text{ads\_mm}}(\theta(O))$  dependencies and thermodynamical preferences: (i) decreasing  $E_{\text{ads\_mm}}(\theta(O))$  and heterogeneous distribution of O atoms (stoichiometric oxide + metal; e.g. Al or La), (ii) increasing  $E_{\text{ads\_mm}}(\theta(O))$  and homogeneous distribution of O atoms (substoichiometric oxide; e.g. Ti or Zr), (iii) concave  $E_{\text{ads\_mm}}(\theta(O))$  and homogeneous distribution of O atoms at low  $\theta(O)$  and heterogeneous at high  $\theta(O)$  (e.g. Sc or Y), etc. This is of crucial importance for the quantities such as secondary electron emission yield, which are guaranteed to correspond to a weighted average of those of stoichiometric oxide and metal only in the case of heterogeneous O atom distribution. The results are correlated with formation enthalpies of oxides of various compositions, surface atomic densities of individual metals, and experimental results such as the time dependence of the magnetron voltage during sputter cleaning of oxidized metal targets. Furthermore, we demonstrate use of these results by presenting static and dynamic Monte Carlo simulations of sputtering.

**Accession Number:** WOS:000528843600007

**Author Identifiers:**

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

ISSN: 0257-8972

**Record 68 of 236**

**Title:** Molecular Force Field Development for Aqueous Electrolytes: 2. Polarizable Models Incorporating Crystalline Chemical Potential and Their Accurate Simulations of Halite, Hydrohalite, Aqueous Solutions of NaCl, and Solubility

**Author(s):** Dockal, J (Dockal, Jan); Lisal, M (Lisal, Martin); Moucka, F (Moucka, Filip)

**Source:** JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 16 Issue: 6 Pages: 3677-3688 DOI: 10.1021/acs.jctc.0c00161 Published: JUN 9 2020

**Abstract:** The current state-of-the-art force fields (FFs) for Na<sup>+</sup> and Cl<sup>-</sup> ions are not capable of simultaneously predicting the thermodynamic properties of the aqueous solution and the crystalline phase. This is primarily due to an oversimplification of the interaction models used but partially also due to the insufficient parametrization of the FFs. We have devised a straightforward and simple parametrization procedure for determining the ion-ion interaction parameters in complex molecular models of NaCl electrolytes which involves fitting the density, lattice energy, and chemical potential of crystalline NaCl at ambient conditions. Starting from the AH/ BK3 and MAH/BK3 FFs, the parametrization approach is employed to develop a complex and accurate polarizable molecular model for the NaCl electrolyte by parametrizing the ion-ion interactions. The performance of the refined polarizable NaCl FF is assessed by evaluating the different thermodynamic and mechanical properties of the crystal, density of crystalline and molten NaCl, along with the melting temperature, properties of aqueous solutions, and the structure and stability of hydrohalite. The simulation results confirm the superiority of the refined FF in comparison with the existing state-of-the-art FFs to accurately predict a wide range of system properties in different NaCl phases, including NaCl aqueous solubility. The refined FF may find applications in the accurate simulations of NaCl electrolytes including inhomogeneous environment, phase equilibria and interfaces, and metastable states. Finally, the parametrization strategy is robust and general and can be used to devise molecular models for other electrolytes.

**Accession Number:** WOS:000541503600020

**PubMed ID:** 32396723

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Moucka, Filip	M-4013-2013	0000-0002-1400-7890
Lisal, Martin	A-8176-2011	0000-0001-8005-7143
Dockal, Jan		0000-0003-0551-0694

ISSN: 1549-9618

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**Record 69 of 236**

**Title:** Heads or Tails? Sandwich-Type Metallo Complexes of Hexakis(2,3-di-O-methyl)-alpha-cyclodextrin

**Author(s):** Jurcek, O (Jurcek, Ondrej); Puttreddy, R (Puttreddy, Rakesh); Topic, F (Topic, Filip); Jurcek, P (Jurcek, Pia); Zarabadi-Poor, P (Zarabadi-Poor, Pezhman); Schroder, HV (Schroder, Hendrik, V); Marek, R (Marek, Radek); Rissanen, K (Rissanen, Kari)

**Source:** CRYSTAL GROWTH & DESIGN Volume: 20 Issue: 6 Pages: 4193-4199 DOI: 10.1021/acs.cgd.0c00532 Published: JUN 3 2020

**Abstract:** Native and synthetically modified cyclodextrins (CDs) are useful building blocks in the construction of large coordination complexes and porous materials with various applications. Sandwich-type complexes (STCs) are one of the important groups in this area. Usually, coordination of secondary hydroxyls or the "head" portal of native CD molecules to a notional multinuclear ring of metal cations leads to formation of head-to-head STCs. Our study introduces a new CD ligand, hexakis(2,3-di-O-methyl)-alpha-cyclodextrin, which enables formation of not only intriguing head-to-head but also novel tail-to-tail STCs. Homometallic silver-based head-to-head STCs, AgPF<sub>6</sub>-STC and AgClO<sub>4</sub>-STC, were obtained by coordination of ligand methoxy groups to six Ag<sup>+</sup>, while bulky counteranions are not only located on the outside but also fill the inner space of the infinite linear channels formed. In contrast, the unique homometallic tail-to-tail RbF<sup>-</sup>-STC was prepared by complexation of primary hydroxyls, "tails", to 12 Rb<sup>+</sup> cations tightly interconnected by 12 F<sup>-</sup> anions, creating a complex structure with accessible pores for potential gas adsorption.

**Accession Number:** WOS:000538515500071

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Rissanen, Kari T	B-5688-2008	0000-0002-7282-8419
Jurcek, Pia	C-7788-2018	0000-0003-4372-9187
Marek, Radek	D-6929-2012	0000-0002-3668-3523
Jurcek, Ondrej	P-5190-2015	0000-0002-9809-656X
Zarabadi-Poor, Pezhman	A-6362-2011	0000-0002-6377-7592
Puttreddy, Rakesh	L-3026-2017	0000-0002-2221-526X
Topic, Filip	O-3059-2015	0000-0003-3811-6036

ISSN: 1528-7483

eISSN: 1528-7505

**Record 70 of 236**

**Title:** Electrical transport properties of bulk tetragonal CuMnAs

**Author(s):** Volny, J (Volny, J.); Wagenknecht, D (Wagenknecht, D.); Zelezny, J (Zelezny, J.); Harcuba, P (Harcuba, P.); Duverger-Nedellec, E (Duverger-Nedellec, E.); Colman, RH (Colman, R. H.); Kudrnovsky, J (Kudrnovsky, J.); Turek, I (Turek, I.); Uhlirva, K (Uhlirva, K.); Vyborny, K (Vyborny, K.)

**Source:** PHYSICAL REVIEW MATERIALS Volume: 4 Issue: 6 Article Number: 064403 DOI: 10.1103/PhysRevMaterials.4.064403 Published: JUN 1 2020

**Abstract:** Temperature-dependent resistivity  $\rho(T)$  and magnetoresistance are measured in bulk tetragonal phase of antiferromagnetic CuMnAs and are found to be anisotropic both due to structure and magnetic order. We compare these findings to model calculations with chemical disorder and finite-temperature phenomena included. The finite-temperature ab initio calculations are based on the alloy analogy model implemented within the coherent potential approximation and the results are in fair agreement with experimental data. Regarding the anisotropic magnetoresistance (AMR), which reaches a modest magnitude of 0.12%, we phenomenologically employ the Stoner-Wohlfarth model to identify temperature-dependent magnetic anisotropy of our samples and conclude that the field dependence of AMR is more similar to that of antiferromagnets than ferromagnets, suggesting that the origin of AMR is not related to isolated Mn magnetic moments.

**Accession Number:** WOS:000537212000006

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Colman, Ross H	C-1657-2017	0000-0002-5039-9764
Zelezny, Jakob	G-5276-2014	0000-0001-9471-0078
Duverger-Nedellec, Elen		0000-0002-3988-6115
Turek, Iija	G-5553-2014	0000-0002-0604-6590
Volny, Jiri		0000-0003-1329-9120
Uhlirva, Klara	C-8505-2013	0000-0002-6889-3621
Harcuba, Petr	P-6279-2016	0000-0002-9910-9158



ISSN: 2475-9953

## Record 71 of 236

**Title:** Regular Two-Dimensional Arrays of Surface-Mounted Molecular Switches: Switching Monitored by UV-vis and NMR Spectroscopy**Author(s):** Hurtado, CS (Hurtado, Carina Santos); Bastien, G (Bastien, Guillaume); Masat, M (Masat, Milan); Stoczek, JR (Stoczek, Jakub Radek); Dracinsky, M (Dracinsky, Martin); Roncevic, I (Roncevic, Igor); Cisarova, I (Cisarova, Ivana); Rogers, CT (Rogers, Charles T.); Kaleta, J (Kaleta, Jiri)**Source:** JOURNAL OF THE AMERICAN CHEMICAL SOCIETY Volume: 142 Issue: 20 Pages: 9337-9351 DOI: 10.1021/jacs.0c01753 Published: MAY 20 2020**Abstract:** Using solid-state N-15 NMR spectroscopy, the cis/trans isomerization in a two-dimensional (2-D) array of surface-mounted azobenzene-based switches was detected for the first time. In order to achieve this, a new class of rod-shaped molecular switches, suitable for formation of 2-D regular arrays on large facets of tris(o-phenylenedioxy)cyclotriphosphazene (TPP) nanocrystals, was synthesized. A mechanochemical approach was used to prepare corresponding host-guest surface inclusions in a TPP matrix. Comparison of thermal steps in solution and supramolecular surface inclusions revealed that switching of individual molecules is not compromised by the close proximity of neighbors.**Accession Number:** WOS:000537415600030**PubMed ID:** 32330034**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Roncevic, Igor	ABH-3076-2020	0000-0003-2175-8059
Roncevic, Igor	ABA-5332-2020	
Cisarova, Ivana	B-1385-2017	0000-0002-9612-9831
Dracinsky, Martin	B-5813-2013	0000-0002-4495-0070
Kaleta, Jiri	D-7405-2014	0000-0002-5561-7580
ROGERS, CHARLES		0000-0002-2278-6863

ISSN: 0002-7863

eISSN: 1520-5126

## Record 72 of 236

**Title:** Photochemical Oxidation Specific to Distorted Aromatic Amines Providing ortho-Diketones**Author(s):** Jakubec, M (Jakubec, Martin); Hansen-Trooyen, S (Hansen-Trooyen, Susanne); Cisarova, I (Cisarova, Ivana); Sykora, J (Sykora, Jan); Storch, J (Storch, Jan)**Source:** ORGANIC LETTERS Volume: 22 Issue: 10 Pages: 3905-3910 DOI: 10.1021/acs.orglett.0c01190 Published: MAY 15 2020**Abstract:** A straightforward visible-light-promoted oxidation of aminohelicenes providing helical ortho-diketones is described. It is shown that the oxidation of amines proceeds via [2 + 2]-cycloaddition reaction with singlet oxygen as an oxidizer and the reaction is specific to distorted aromatic systems. The versatility of the prepared diketones and tetraketones was proven in several heterocycle-forming reactions. The observed adjustment of the physicochemical properties of original molecules is valuable for further development of functional molecules based on helicenes.**Accession Number:** WOS:000535292300034**PubMed ID:** 32352305**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Cisarova, Ivana	B-1385-2017	0000-0002-9612-9831
Jakubec, Martin		0000-0001-7377-9359

ISSN: 1523-7060

eISSN: 1523-7052

## Record 73 of 236

**Title:** Bixbyite-Ta<sub>2</sub>N<sub>2</sub>O film prepared by HiPIMS and postdeposition annealing: Structure and properties**Author(s):** Capek, J (Capek, J.); Batkova, S (Batkova, S.); Matas, M (Matas, M.); Kos, S (Kos, S.); Kozak, T (Kozak, T.); Haviar, S (Haviar, S.); Houska, J (Houska, J.); Schusser, J (Schusser, J.); Minar, J (Minar, J.); Dvorak, F (Dvorak, F.); Zeman, P (Zeman, P.)**Source:** JOURNAL OF VACUUM SCIENCE & TECHNOLOGY A Volume: 38 Issue: 3 Article Number: 033409 DOI: 10.1116/6.0000066 Published: MAY 2020**Abstract:** High-power impulse magnetron sputtering of a Ta target in precisely controlled Ar

+O

2 +N

2 gas mixtures was used to prepare amorphous N-rich tantalum oxynitride (Ta-O-N) films with a finely varied elemental composition. Postdeposition annealing of the films at 900

degrees C for 5 min in vacuum led to their crystallization without any significant change in the elemental composition. The authors show that this approach allows preparation of a Ta-O-N film with a dominant Ta

2N

2O phase of the bixbyite structure. As far as the authors know, this phase has been neither experimentally nor theoretically reported yet. The film exhibits semiconducting properties characterized by two electrical (indirect or selection-rule forbidden) bandgaps of about 0.2 and 1.0 eV and one optical (direct and selection-rule allowed) bandgap of 2.0 eV (suitable for visible-light absorption up to 620 nm). This observation is in good agreement with the carried out ab initio calculations and the experimental data obtained by soft and hard X-ray photoelectron spectroscopy. Furthermore, the optical bandgap is appropriately positioned with respect to the redox potentials for water splitting, which makes this material an interesting candidate for this application.

**Accession Number:** WOS:000529406300001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Capek, Jiri	F-9784-2016	0000-0002-3267-7708
Minar, Jan	O-3186-2013	0000-0001-9735-8479
Zeman, Petr	B-9252-2016	0000-0001-8742-4487

ISSN: 0734-2101

eISSN: 1520-8559

## Record 74 of 236

**Title:** Anisotropy of resistivity in hexagonal late transition metals and their alloys**Author(s):** Wagenknecht, D (Wagenknecht, D.); Turek, I (Turek, I)**Source:** JOURNAL OF PHYSICS-CONDENSED MATTER Volume: 32 Issue: 18 Article Number: 185802 DOI: 10.1088/1361-648X/ab6d17 Published: MAY 1 2020**Abstract:** Transport properties of hexagonal transition metals Co, Ru, and Os at finite temperatures are studied by means of ab initio electronic structure techniques and the Kubo linear response theory. An alloy analogy model for a quantitative treatment of the electrical conductivities due to temperature-induced lattice vibrations (phonons) and spin fluctuations is applied with focus on anisotropy induced by the hexagonal structure. The resistivity anisotropy in Co is found opposite to that in Ru and Os, in agreement with existing experimental data. This result is ascribed to the strong itinerant ferromagnetism of Co which leads to profound differences in the electronic structure and conductivities in the majority and minority spin channels. A similar sensitivity to spin polarization is predicted for the anisotropy of residual resistivity in random hexagonal Co-rich Co-Ni and Co-Ni-Fe alloys.**Accession Number:** WOS:000524296200002**PubMed ID:** 31952057**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Wagenknecht, David	P-4165-2017	0000-0003-1927-9702

ISSN: 0953-8984

eISSN: 1361-648X

**Record 75 of 236****Title:** Azomethine phthalimides fluorescent E -> Z photoswitches**Author(s):** Georgiev, A (Georgiev, Anton); Yordanov, D (Yordanov, Dancho); Dimov, D (Dimov, Deyan); Zhivkov, I (Zhivkov, Ivailo); Nazarova, D (Nazarova, Dimana); Weiter, M (Weiter, Martin)**Source:** JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A-CHEMISTRY **Volume:** 393 **Article Number:** 112443 **DOI:** 10.1016/j.jphotochem.2020.112443 **Published:** APR 15 2020

**Abstract:** Herein, we report the synthesis and E -> Z photoswitching behavior of two 4-substituted azomethine phthalimides containing anthracenyl and 4-(dimethylamino)phenyl moieties (EAMP1 and EAMP2). These compounds represent newly synthesized and unstudied photoswitches with dual fluorescence properties as E-isomers and at photostationary state (PSS) depending on the solvent polarity. Steady-state fluorescence measurements were performed in various solvents and the results show strong sensitivity on the environmental polarity. The kinetics of E -> Z photoswitching to PSS was studied in AcCN by visible light activation at 410 nm (EAMP1) and long wavelength UV-light activation at 350 nm (EAMP2). The quantitative and qualitative performance of the switching behavior was evaluated by the degree of photoisomerization (R) and the rate constant (k). It was found for EAMP1 R = 6.95 %, k = 8.87 x 10<sup>(-4)</sup> s<sup>(-1)</sup> and EAMP2 R = 88.72 %, k = 4.00 x 10<sup>(-4)</sup> s<sup>(-1)</sup>, respectively. The reason for the lower photoconversion of EAMP1 compared to the EAMP2 was analyzed through optimization of the molecular geometry of E- and Z-isomers in the ground state (S-0) and first excited state (S-1) by DFT/TD-DFT calculations with B3LYP/6-31 + G(d,p) level of theory using IEFPCM in AcCN. It was found that E-isomers in the S-0 have nonplanar conformation, while the Z-isomer of EAMP1 prefers twisted conformation and the Z-isomer of EAMP2 T-shaped conformation is energetically advantageous compared to the twisted one. The reason is the weak H.....pi noncovalent interaction (NCI) between 4-(dimethylamino)phenyl moiety and phthalimide ring. Moreover, the Z-isomer of EAMP2 is unusual stable up to 600 min at room temperature in dark compared to the EAMP1, which undergoes full Z -> E relaxation for less than 60 min at the same conditions. The Z -> E relaxation of EAMP2 is achieved for 90 min at 60 degrees C. The fluorescence E -> Z switching behavior was studied by emission measurements in AcCN and 1,4-DOX as E-isomers and at PSS in room and liquid nitrogen (77 K) temperatures. In the polar and nonpolar solvents, red-shifted emissions with increased fluorescence quantum (Phi(f)) yields have been observed at PSS compared to the E-isomers. The molecular rotor behavior was studied in the binary mixture of glycerol:ethanol and the results show a sensitivity of the emission bands depending on the environmental viscosity. Time-resolved fluorescence decay measurements were performed in AcCN and 1,4-DOX as E-isomers and at PSS to estimate the mechanism of fundamental fluorescence bands. We found that dyes at PSS have longer lifetime (tau) compared to the E-isomers, especially in less polar 1,4-DOX.

**Accession Number:** WOS:000528279200010**ISSN:** 1010-6030**Record 76 of 236****Title:** Efficient Estimation of Absolute Binding Free Energy for a Homeodomain-DNA Complex from Nonequilibrium Pulling Simulations**Author(s):** Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri)**Source:** JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 16 **Issue:** 4 **Pages:** 2034-2041 **DOI:** 10.1021/acs.jctc.0c00006 **Published:** APR 14 2020

**Abstract:** Estimation of binding free energies is one of the central aims of simulations of biomolecular complexes. We explore the accuracy and efficiency of setups based on nonequilibrium pulling simulations applied to the estimation of binding affinities of DNA-binding proteins. Absolute binding free energies are calculated over a range of temperatures and compared to results obtained previously using an equilibrium method. We show that realistic binding affinities can be obtained with the presented nonequilibrium approach, which also entails lower computational requirements. Errors of the binding free energy estimates are investigated and are shown to be comparable to those observed previously. Bounds are provided on the convergence of the errors with respect to the number of pulling simulations performed and with respect to the applied pull rate.

**Accession Number:** WOS:000526313000004**PubMed ID:** 32208691**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
vondrasek, jiri		0000-0002-6066-973X

**ISSN:** 1549-9618**eISSN:** 1549-9626**Record 77 of 236****Title:** Conformation in Ultrathin Polymer Brush Coatings Resolved by Infrared Nanoscopy**Author(s):** Pereira, AD (Pereira, Andres de los Santos); Cernescu, A (Cernescu, Adrian); Svoboda, J (Svoboda, Jan); Sivkova, R (Sivkova, Radoslava); Romanenko, I (Romanenko, Iryna); Bashta, B (Bashta, Bogdana); Keilmann, F (Keilmann, Fritz); Pop-Georgievski, O (Pop-Georgievski, Ognen)**Source:** ANALYTICAL CHEMISTRY **Volume:** 92 **Issue:** 7 **Pages:** 4716-4720 **DOI:** 10.1021/acs.analchem.9b05661 **Published:** APR 7 2020

**Abstract:** Polymer brush coatings are effective in preventing blood coagulation or bacterial attachment, but their chain conformation, while vital for this effect, was never characterized in high spatial resolution. Here, we report mid-infrared spectroscopic nanoscopy studies of few-nanometer-thin poly(ethylene oxide) (PEO) films which reveal marked spectral variations along the surface at a length scale smaller than 100 nm and originating only from the physical conformation of the chains. The conformation and average orientation of the polymer chains in the layer is extracted from the spectra with the aid of theoretic modeling, confirming the spontaneous formation of a crystalline phase. This result suggests spectroscopic nanoscopy as a powerful new tool to characterize polymer brush coatings.

**Accession Number:** WOS:000526569200005**PubMed ID:** 32129604**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Bashta, Bogdana	AAD-6604-2020	0000-0002-5592-8370
Svoboda, Jan	E-4750-2014	0000-0002-4989-4274
Pop-Georgievski, Ognen	G-3498-2014	0000-0001-7938-9271
de los Santos Pereira, Andres	G-5141-2014	0000-0002-0138-1357

**ISSN:** 0003-2700**eISSN:** 1520-6882**Record 78 of 236****Title:** Elimination of Viroids from Tobacco Pollen Involves a Decrease in Propagation Rate and an Increase of the Degradation Processes**Author(s):** Matousek, J (Matousek, Jaroslav); Steinbachova, L (Steinbachova, Lenka); Drabkova, LZ (Zaveska Drabkova, Lenka); Kocabek, T (Kocabek, Tomas); Potesil, D (Potesil, David); Mishra, AK (Mishra, Ajay Kumar); Honys, D (Honys, David); Steger, G (Steger, Gerhard)**Source:** INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES **Volume:** 21 **Issue:** 8 **Article Number:** 3029 **DOI:** 10.3390/ijms21083029 **Published:** APR 2020

**Abstract:** Some viroids-single-stranded, non-coding, circular RNA parasites of plants-are not transmissible through pollen to seeds and to next generation. We analyzed the cause for the elimination of apple fruit crinkle viroid (AFCVd) and citrus bark cracking viroid (CBCVd) from male gametophyte cells of Nicotiana tabacum by RNA deep sequencing and molecular methods using infected and transformed tobacco pollen tissues at different developmental stages. AFCVd was not transferable from pollen to seeds in reciprocal pollinations, due to a complete viroid eradication during the last steps of pollen development and fertilization. In pollen, the viroid replication pathway proceeds with detectable replication intermediates, but is dramatically depressed in comparison to leaves. Specific and unspecific viroid degradation with some preference for (-) chains occurred in pollen, as detected by analysis of viroid-derived small RNAs, by quantification of viroid levels and by detection of viroid degradation products forming "comets" on Northern blots. The decrease of viroid levels during pollen development correlated with mRNA accumulation of several RNA-degrading factors, such as AGO5 nuclease, DICER-like and TUDOR S-like nuclease. In addition, the functional status of pollen, as a tissue with high ribosome content, could play a role during suppression of AFCVd replication involving transcription factors IIIA and ribosomal protein L5.

**Accession Number:** WOS:000535565300371**PubMed ID:** 32344786**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Potesil, David	D-9696-2012	0000-0003-0390-0904
Kocabek, Tomas	G-9506-2014	0000-0002-4621-4181
Drabkova, Lenka Zaveska	F-6999-2012	0000-0003-1140-6607
Mishra, Ajay Kumar	J-8857-2014	
Matousek, Jaroslav	G-8576-2014	
Steinbachova, Lenka		0000-0001-8347-5770

Matousek, Jaroslav 0000-0002-7490-9108

eISSN: 1422-0067

**Record 79 of 236****Title:** Phylogenomic insights into the Fascicularia-Ochagavia group (Bromelioideae, Bromeliaceae)**Author(s):** Paule, J (Paule, Juraj); Schmickl, R (Schmickl, Roswitha); Fer, T (Fer, Tomas); Matuszak-Renger, S (Matuszak-Renger, Sabine); Halbritter, H (Halbritter, Heidemarie); Zizka, G (Zizka, Georg)**Source:** BOTANICAL JOURNAL OF THE LINNEAN SOCIETY **Volume:** 192 **Issue:** 4 **Special Issue:** SI **Pages:** 642-655 **DOI:** 10.1093/botlinnean/boz085 **Published:** APR 2020**Abstract:** Ochagavia (four species) and Fascicularia (one species) form a well-supported clade of the early-diverging Bromelioideae. The two genera are morphologically similar, but they can be easily discerned on the basis of generative characters. Besides the species distributed on the Chilean mainland, the group includes *O. elegans*, endemic to the Robinson Crusoe Island of the Juan Fernandez Islands. In previous molecular phylogenetic studies, *O. elegans* formed a sister clade to the remainder of Fascicularia and Ochagavia. A phylogenomic approach, including nearly complete and, in five cases, full plastomes (c. 160 kbp) and the nuclear rDNA cistron (c. 6 kbp), and scanning electron microscope (SEM) images of pollen were used to analyse relationships in the Fascicularia-Ochagavia group. Plastome and nuclear trees were largely congruent and supported previous phylogenetic analyses of *O. elegans* being sister to the remainder of the group. A divergent phylogenetic position was suggested for *O. carnea* using different organellar trees. SEM analysis of pollen supported the division of Fascicularia and Ochagavia. Evolutionary and taxonomic implications of our results are discussed.**Accession Number:** WOS:000537361100007**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Paule, Juraj	A-2998-2017	0000-0001-5375-7689
Fer, Tomas	A-9991-2008	0000-0002-0126-3684

ISSN: 0024-4074

eISSN: 1095-8339

**Record 80 of 236****Title:** Dependence of amino-acid dielectric relaxation on solute-water interaction: Molecular dynamics study**Author(s):** Prusa, J (Prusa, Jiri); Cifra, M (Cifra, Michal)**Source:** JOURNAL OF MOLECULAR LIQUIDS **Volume:** 303 **Article Number:** 112613 **DOI:** 10.1016/j.molliq.2020.112613 **Published:** APR 1 2020**Abstract:** Computational molecular methods represent an ultimate microscope to visualize and quantify dynamics of biomolecules and nanostructures on the atomic scale and also a tool to link this dynamics to macroscopic observables.

However, these potentially powerful computational methods have been so far poorly explored to gain a deeper knowledge of broadband biomolecular dielectric properties which are essential for novel noninvasive electromagnetic methods in biomedical diagnostics and treatment.

To fill in this gap, we explore here a broad range of parameter space of molecular dynamics simulation (two common water models, four force fields, eight types of amino acids) and demonstrate their effects on dielectric increment and relaxation time. We found that the force field and water parameters influence the extracted dielectric increment and relaxation time of the biomolecule-water solution dielectric spectra significantly. To understand this observation, we dissected the effect of individual parameters of molecular force field on the dielectric spectra. For the first time, we showed the charges on the atoms, and the bond length of amino acids are the determining factors of both their dielectric increment and relaxation time in molecular dynamics simulations.

Hence, our results leverage atomic resolution-based computational methods for a deeper understanding of biomolecular microwave dielectric properties with potential biological, medical and nanotechnological applications. (C) 2020 Elsevier B.V. All rights reserved.

**Accession Number:** WOS:000533612700006

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eISSN: 1873-3166

**Record 81 of 236****Title:** Identification of the most active sites for tetrahydropyranlation in zeolites: MFI as a test case**Author(s):** Liu, M (Liu, Mingxiu); Vesely, O (Vesely, Ondrej); Eliasova, P (Eliasova, Pavla); Shamzhy, M (Shamzhy, Mariya); Lyu, P (Lyu, Pengbo); Grajciar, L (Grajciar, Lukas)**Source:** CATALYSIS TODAY **Volume:** 345 **Special Issue:** SI **Pages:** 165-174 **DOI:** 10.1016/j.cattod.2019.08.017 **Published:** APR 1 2020**Abstract:** Tetrahydropyranlation (THP) has been extensively studied experimentally with both Bronsted and Lewis acid-based catalysts, such as zeolites, considered. However, our atomic-level understanding of the underlying mechanisms of different types of catalytic sites remains limited, particularly regarding zeolites. Thus, we combined an experimental catalytic study with density functional theory (DFT) calculations to identify the active sites and corresponding reaction mechanism in MFI zeolite. Both experimental and computational data clearly show that Bronsted acid sites are more reactive than Lewis acid sites. Furthermore, calculated reaction barriers for Bronsted acid site catalysis (5 kcal mol<sup>-1</sup>) are much lower than those for the diffusion of bulky products in microporous channels (approximately 20 kcal mol<sup>-1</sup>). In full agreement with theoretical calculations, the results of Madon-Boudart test clearly show that the effect of diffusion on the H-MFI catalysts performance cannot be neglected even at low temperature. Therefore, the diffusion becomes the rate-determining step. Overall, our findings suggest that designing zeolites with improved THP catalysis performance requires focusing on acid zeolites with Bronsted acid sites of average strength with facilitated diffusion, e.g., due to auxiliary mesoporous system.**Accession Number:** WOS:000522039100019**Conference Title:** 8th Czech-Italian-Spanish Symposium on Zeolites and Catalysis**Conference Date:** JUN, 2019**Conference Location:** Amantea, ITALY**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lyu, Pengbo	O-9415-2017	0000-0002-1785-9861
Shamzhy, Mariya	F-5477-2014	0000-0002-1979-6817
Vesely, Ondrej	M-6986-2017	0000-0002-8350-7725
Grajciar, Lukas	H-1266-2015	0000-0001-9464-7769

ISSN: 0920-5861

eISSN: 1873-4308

**Record 82 of 236****Title:** How spin-orbital entanglement depends on the spin-orbit coupling in a Mott insulator**Author(s):** Gotfryd, D (Gotfryd, Dorota); Parschke, EM (Parschke, Ekaterina M.); Chaloupka, J (Chaloupka, Jiff); Oles, AM (Oles, Andrzej M.); Wohlfeld, K (Wohlfeld, Krzysztof)**Source:** PHYSICAL REVIEW RESEARCH **Volume:** 2 **Issue:** 1 **Article Number:** 013353 **DOI:** 10.1103/PhysRevResearch.2.013353 **Published:** MAR 20 2020**Abstract:** The concept of the entanglement between spin and orbital degrees of freedom plays a crucial role in our understanding of various phases and exotic ground states in a broad class of materials, including orbitally ordered materials and spin liquids. We investigate how the spin-orbital entanglement in a Mott insulator depends on the value of the spin-orbit coupling of the relativistic origin. To this end, we numerically diagonalize a one-dimensional spin-orbital model with Kugel-Khomskii exchange interactions between spins and orbitals on different sites supplemented by the on-site spin-orbit coupling. In the regime of small spin-orbit coupling with regard to the spin-orbital exchange, the ground state to a large extent resembles the one obtained in the limit of vanishing spin-orbit coupling. On the other hand, for large spin-orbit coupling the ground state can, depending on the model parameters, either still show negligible spin-orbital entanglement or evolve to a highly spin-orbitally-entangled phase with completely distinct properties that are described by an effective XXZ model. The presented results suggest that (i) the spin-orbital entanglement may be induced by large on-site spin-orbit coupling, as found in the 5d transition metal oxides, such as the iridates; (ii) for Mott insulators with weak spin-orbit coupling of Ising type, such as, e.g., the alkali hyperoxides, the effects of the spin-orbit coupling on the ground state can, in the first order of perturbation theory, be neglected.**Accession Number:** WOS:000602699300009**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Wohlfeld, Krzysztof	Q-2351-2019	0000-0002-6524-8264
Chaloupka, Jiri		0000-0001-8898-0442
Paerschke, Ekaterina		0000-0003-0853-8182
Oles, Andrzej M.		0000-0002-8954-3233



Gotfryd, Dorota 0000-0002-4496-5619

eISSN: 2643-1564

**Record 83 of 236****Title:** Oxidation Enhances Aerosol Nucleation: Measurement of Kinetic Pickup Probability of Organic Molecules on Hydrated Acid Clusters**Author(s):** Lengyel, J (Lengyel, Jozef); Pysanenko, A (Pysanenko, Andriy); Farnikova, K (Farnikova, Karolina); Pluharova, E (Pluharova, Eva); Farnik, M (Farnik, Michal)**Source:** JOURNAL OF PHYSICAL CHEMISTRY LETTERS **Volume:** 11 **Issue:** 6 **Pages:** 2101-2105 **DOI:** 10.1021/acs.jpcllett.0c00207 **Published:** MAR 19 2020**Abstract:** We investigate the uptake of the most prominent biogenic volatile organic compounds (VOCs)-isoprene, a-pinene, and their selected oxidation products-by hydrated acid clusters in a molecular beam experiment and by DFT calculations. Our experiments provide a unique and direct way of determination of the surface accommodation coefficient ( $\alpha(S)$ ) on the proxies of ultrafine aerosol particles. Since we are able to determine unambiguously the fraction of the clusters to which the molecules stick upon collisions, our  $\alpha(S)$  is a purely kinetic parameter disentangling the molecule pickup from its evaporation. Oxidation increases the  $\alpha(S)$  of VOCs by more than an order of magnitude, because oxidized compounds form hydrogen bonds with the clusters, whereas the interactions of the parent VOCs are weaker and nonspecific. This work provides molecular-level insight into the condensation of single molecules into atmospheric particles, which has important implications for aerosol nucleation and growth.**Accession Number:** WOS:000526339000018**PubMed ID:** 32101439**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pluharova, Eva	B-1092-2012	
Lengyel, Jozef	B-9987-2012	0000-0002-1971-2783
Farnik, Michal	F-5274-2014	0000-0002-7106-0719
Pluharova, Eva		0000-0002-4167-4891

ISSN: 1948-7185

**Record 84 of 236****Title:** Quantum dissipation driven by electron transfer within a single molecule investigated with atomic force microscopy**Author(s):** Berger, J (Berger, Jan); Ondracek, M (Ondracek, Martin); Stetsovych, O (Stetsovych, Oleksandr); Maly, P (Maly, Pavel); Holy, P (Holy, Petr); Rybacek, J (Rybacek, Jiri); Svec, M (Svec, Martin); Stara, IG (Stara, Irena G.); Mancal, T (Mancal, Tomas); Stary, I (Stary, Ivo); Jelinek, P (Jelinek, Pavel)**Source:** NATURE COMMUNICATIONS **Volume:** 11 **Issue:** 1 **Article Number:** 1337 **DOI:** 10.1038/s41467-020-15054-w **Published:** MAR 12 2020**Abstract:** Intramolecular charge transfer processes play an important role in many biological, chemical and physical processes including photosynthesis, redox chemical reactions and electron transfer in molecular electronics. These charge transfer processes are frequently influenced by the dynamics of their molecular or atomic environments, and they are accompanied with energy dissipation into this environment. The detailed understanding of such processes is fundamental for their control and possible exploitation in future technological applications. Most of the experimental studies of the intramolecular charge transfer processes so far have been carried out using time-resolved optical spectroscopies on large molecular ensembles. This hampers detailed understanding of the charge transfer on the single molecular level. Here we build upon the recent progress in scanning probe microscopy, and demonstrate the control of mixed valence state. We report observation of single electron transfer between two ferrocene redox centers within a single molecule and the detection of energy dissipation associated with the single electron transfer.**Accession Number:** WOS:000563527200001**PubMed ID:** 32165626**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Svec, Martin	ABA-1323-2020	0000-0003-0369-8144
Jelinek, Pavel	ABE-8589-2020	0000-0002-5645-8542
Svec, Martin	G-6645-2014	0000-0003-0369-8144
Ondracek, Martin		0000-0002-8808-1487
Stetsovych, Oleksandr		0000-0001-7788-1617
Mancal, Tomas	B-9688-2014	0000-0003-1736-3054

ISSN: 2041-1723

**Record 85 of 236****Title:** Formation of CO+ by radiative association II**Author(s):** Zamecnikova, M (Zamecnikova, Martina); Gustafsson, M (Gustafsson, Magnus); Nyman, G (Nyman, Gunnar); Soldan, P (Soldan, Pavel)**Source:** MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY **Volume:** 492 **Issue:** 3 **Pages:** 3794-3802 **DOI:** 10.1093/mnras/stz3641 **Published:** MAR 2020**Abstract:** Radiative association of an oxygen atom with a carbon cation is investigated using quantal and semiclassical methods. The total rate coefficient for spontaneous radiative association of O(2s(2)2p(4), P-3) with C+(2s(2)2p, P-2) on the doublet manifold is determined from the corresponding cross-sections. The cross-sections for the 1(2) Sigma(-) -> A(2)Pi, 2(2) Sigma(-) -> A(2)Pi, and C-2 Delta -> A(2)Pi continuum-bound processes are calculated either semiclassically, in combination with the Breit-Wigner approach, or fully quantum mechanically. In the temperature range 10-10 000 K, our recommended total rate coefficient, obtained from these calculations and the data of Zdeafkova et al. (2019), slowly increases from 7.5 x 10(-18) cm(3)s(-1) to 2.1 x 10(-17) cm(3)s(-1). Corresponding aspects of the CO+ and CO formations in SN 1987A are discussed.**Accession Number:** WOS:000518143200052**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Zamecnikova, Martina	AAP-4710-2020	0000-0003-1619-3583
Gustafsson, Magnus	A-1661-2010	0000-0002-7629-0169
Soldan, Pavel	C-2256-2008	0000-0002-6281-7599

ISSN: 0035-8711

eISSN: 1365-2966

**Record 86 of 236****Title:** Newly identified DNA methyltransferases of Ixodes ricinus ticks**Author(s):** Kotsarenko, K (Kotsarenko, Kateryna); Vechtova, P (Vechtova, Pavlina); Hammerova, Z (Hammerova, Zuzana); Langova, N (Langova, Natalia); Malinovska, L (Malinovska, Lenka); Wimmerova, M (Wimmerova, Michaela); Sterba, J (Sterba, Jan); Grubhoffer, L (Grubhoffer, Libor)**Source:** TICKS AND TICK-BORNE DISEASES **Volume:** 11 **Issue:** 2 **Article Number:** 101348 **DOI:** 10.1016/j.ttbdis.2019.101348 **Published:** MAR 2020**Abstract:** DNA methylation at the fifth position of cytosine (5mC) and at the sixth position of adenine (6mA) plays an important role in the regulation of the gene expression and, in eukaryotes, is essential for normal development. For Ixodes ricinus, the most common European arthropod vector of human and animal pathogens, the DNA methylation profile and the role of DNA methylation in tick development are still under discussion. Our goal was to analyze the status of I. ricinus DNA methylation at different life stages and identify enzymes that produce this type of DNA modification. We found that 5mC and 6mA are present in I. ricinus genomic DNA at all life stages. In the transcriptome of I. ricinus, we identified the sequences of the putative IrDNMT1, IrDNMT3, and IrDAMT enzymes, and bioinformatic analysis and three-dimensional modeling predicted their DNA methylation activity. This confirms that I. ricinus possesses a complete DNA methylation toolkit. Our results suggest that DNA methylation is important for the physiology and transstadial development of ticks.**Accession Number:** WOS:000509982500020**PubMed ID:** 31812591**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Sterba, Jan	E-9533-2012	0000-0003-1005-1787

ISSN: 1877-959X

eISSN: 1877-9603

**Record 87 of 236****Title:** Role of Oxidized Gly25, Gly29, and Gly33 Residues on the Interactions of A beta(1-42) with Lipid Membranes

**Author(s):** Fatafta, H (Fatafta, Hebah); Poojari, C (Poojari, Chetan); Sayyed-Ahmad, A (Sayyed-Ahmad, Abdallah); Strodel, B (Strodel, Birgit); Owen, MC (Owen, Michael C.)

**Source:** ACS CHEMICAL NEUROSCIENCE **Volume:** 11 **Issue:** 4 **Pages:** 535-548 **DOI:** 10.1021/acscchemneuro.9b00558 **Published:** FEB 19 2020

**Abstract:** Oxidative stress is known to play an important role in the pathogenesis of Alzheimer's disease. Moreover, it is becoming increasingly evident that the plasma membrane of neurons plays a role in modulating the aggregation and toxicity of Alzheimer's amyloid-beta peptide (A beta). In this study, the combined and interdependent effects of oxidation and membrane interactions on the 42 residues long A beta isoform are investigated using molecular simulations. Hamiltonian replica exchange molecular dynamics simulations are utilized to elucidate the impact of selected oxidized glycine residues of A beta 42 on the interactions of the peptide with a model membrane comprised of 70% POPC, 25% cholesterol, and 5% of the ganglioside GM1. The main findings are that, independent of the oxidation state, A beta prefers binding to GM1 over POPC, which is further enhanced by the oxidation of Gly29 and Gly33 and reduced the formation of beta-sheet. Our results suggest that the differences observed in A beta 42 conformations and its interaction with a lipid bilayer upon oxidation originate from the position of the oxidized Gly residue with respect to the hydrophobic sequence of A beta 42 involving the Gly29-XXX-Gly33-XXX-Gly37 motif and from specific interactions between the peptide and the terminal sugar groups of GM1.

**Accession Number:** WOS:000515195800005

**PubMed ID:** 31939658

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Owen, Michael	AAW-4453-2020	
Strodel, Birgit	H-5449-2013	0000-0002-8734-7765
Sayyed-Ahmad, Abdallah		0000-0003-2415-8403
Poojari, Chetan		0000-0001-6575-221X

**ISSN:** 1948-7193

**Record 88 of 236**

**Title:** Effect of helical kink in antimicrobial peptides on membrane pore formation

**Author(s):** Tuerkova, A (Tuerkova, Alzbeta); Kabelka, I (Kabelka, Ivo); Kralova, T (Kralova, Tereza); Sukenik, L (Sukenik, Lukas); Pokorna, S (Pokorna, Sarka); Hof, M (Hof, Martin); Vacha, R (Vacha, Robert)

**Source:** ELIFE **Volume:** 9 **Article Number:** e47946 **DOI:** 10.7554/eLife.47946 **Published:** FEB 18 2020

**Abstract:** Every cell is protected by a semipermeable membrane. Peptides with the right properties, for example antimicrobial peptides (AMPs), can disrupt this protective barrier by formation of leaky pores. Unfortunately, matching peptide properties with their ability to selectively form pores in bacterial membranes remains elusive. In particular, the proline/glycine kink in helical peptides was reported to both increase and decrease antimicrobial activity. We used computer simulations and fluorescence experiments to show that a kink in helices affects the formation of membrane pores by stabilizing toroidal pores but disrupting barrel-stave pores. The position of the proline/glycine kink in the sequence further controls the specific structure of toroidal pore. Moreover, we demonstrate that two helical peptides can form a kink-like connection with similar behavior as one long helical peptide with a kink. The provided molecular-level insight can be utilized for design and modification of pore-forming antibacterial peptides or toxins.

**Accession Number:** WOS:000519949800001

**PubMed ID:** 32167466

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Hof, Martin	F-5134-2014	0000-0003-2884-3037
Tuerkova, Alzbeta		0000-0001-7235-9029

**ISSN:** 2050-084X

**Record 89 of 236**

**Title:** Mechanism of sulfonation-induced chain scission of selectively oxidized polysaccharides

**Author(s):** Munster, L (Munster, L.); Hanulikova, B (Hanulikova, B.); Machovsky, M (Machovsky, M.); Latecka, F (Latecka, F.); Kuritka, I (Kuritka, I.); Vicha, J (Vicha, J.)

**Source:** CARBOHYDRATE POLYMERS **Volume:** 229 **Article Number:** 115503 **DOI:** 10.1016/j.carbpol.2019.115503 **Published:** FEB 1 2020

**Abstract:** Oxidation of polysaccharides to 2,3-dicarboxypolysaccharides is a two-stage process, where selective oxidation by periodate is followed by secondary oxidation by chlorite. Addition of sulfamic acid before the secondary oxidation influences the molecular weight and degree of oxidation of the product. Here, mechanism of sulfamic acid-catalysed chain scission is elucidated for selectively oxidized cellulose and dextrin. Initially, sulfamic acid sulfonates the aldehyde groups of 2,3-dialdehyde polysaccharide. Introduced -SO<sub>3</sub>H groups are in ideal position to protonate the oxygen atom of 1-4' glycosidic bond and to trigger acidic hydrolysis. This can be used to obtain a direct control over the molecular weight of the product. Observed slightly lower degree of oxidation was ascribed to the ability of sulfamic acid to scavenge the hypochlorite and thus protect the intermolecular hemiacetals from oxidation. Usually undesirable hypochlorite thus seems to be necessary for preparation of selectively oxidized polysaccharides with degree of oxidation above 90%.

**Accession Number:** WOS:000501796600076

**PubMed ID:** 31826511

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Vicha, Jan	D-8417-2012	0000-0003-3698-8236
Munster, Lukas	E-2522-2015	0000-0003-1643-2038
Machovsky, Michal	J-1818-2016	0000-0003-4825-968X
Kuritka, Ivo	J-2285-2016	0000-0002-1016-5170

**ISSN:** 0144-8617

**eISSN:** 1879-1344

**Record 90 of 236**

**Title:** Intramolecular micellization and nanopatterning in pH- and thermo-responsive molecular brushes

**Author(s):** Prokacheva, VM (Prokacheva, Varvara M.); Rud, OV (Rud, Oleg V.); Uhlak, F (Uhlak, Filip); Borisov, OV (Borisov, Oleg V.)

**Source:** SOFT MATTER **Volume:** 16 **Issue:** 1 **Pages:** 208-218 **DOI:** 10.1039/c9sm01961h **Published:** JAN 7 2020

**Abstract:** Conformational transitions and nanoscale self-organization triggered in double pH- and thermo-responsive molecular brushes by varying environmental conditions are studied by means of analytical mean-field theory and numerical Scheutjens-Fleer self-consistent field modelling. Such molecular brushes are composed of multiple thermo-responsive side chains end-grafted onto the main chain (backbone) and are capable of acquiring ionic charges via reversible (de)protonation of the monomer units. Competition of long-range Coulomb repulsion with short-range solvophobic interactions leads to complex patterns in the intramolecular self-organization of molecular brushes. In particular, we observed formation of pearl necklace-like structures with multiple dense nanodomains formed by weakly ionized collapsed side chains and stabilized by a fraction protruding into the solution and strongly ionized ones. Such structures are thermodynamically stable in a certain parameter range and can be termed as intramolecular micelles. The stimuli-induced intramolecular nanopatterning occurs via a sequence of quasi-first order phase transitions corresponding to splitting/fusion of collapsed domains accompanied by jumps in the average degree of ionization and macromolecular dimensions. A re-entrant sequence of transitions is observed when the salt concentration is used as a control parameter. These theoretical predictions provide guidelines for design of smart unimolecular devices, for example multicompartment nanocarriers of active substances or nanosensors.

**Accession Number:** WOS:000503491000018

**PubMed ID:** 31774442

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Prokacheva, Varvara		0000-0002-0948-7869

**ISSN:** 1744-683X

**eISSN:** 1744-6848

**Record 91 of 236**

**Title:** Numerical modelling of pump absorption in coiled and twisted double-clad fiber: a prospect for tandem pumped fiber laser

**Author(s):** Grabner, M (Grabner, Martin); Nithyanandan, K (Nithyanandan, Kanagaraj); Peterka, P (Peterka, Pavel); Koska, P (Koska, Pavel); Honzatko, P (Honzatko, Pavel); Jasim, AA (Jasim, Ali A.)

Edited by: Kalli K; Peterka P; Bunge CA

Source: MICRO-STRUCTURED AND SPECIALTY OPTICAL FIBRES VI Book Series: Proceedings of SPIE Volume: 11355 Article Number: 113550W DOI: 10.1117/12.2557230 Published: 2020

**Abstract:** The high-power operation of fiber lasers was enabled mainly by the invention of cladding pumping within a double-clad fiber structure. Various cross-sectional shapes of double-clad fibers as well as unconventional coiling methods have been investigated both experimentally and theoretically in order to enhance the absorption of the multimode-pump. With enhanced pump absorption efficiency, the double-clad fiber of shorter length can be used in the fiber devices and in such a way the unwanted effects of background losses and nonlinear effects can be mitigated. In this paper we report on numerical modelling of optical pump absorption in double-clad octagonal active fiber of different fiber geometry and layouts. Namely we investigate the effect of the bending radii, twist rate of the fiber, doped core area (holmium is considered in this as a doping ion) and pump beam shape. The numerical model is based on FEM-BPM method. The optimized geometries and layouts shall finally result in a highly efficient laser of small footprint without the need of water cooling with great potential for application with low power consumption, tightly limited space and weight requirements. Optimized design will also minimize risk of damage of the fiber during operation of the fiber laser.

Accession Number: WOS:000576761300021

Conference Title: Conference on Micro-Structured and Specialty Optical Fibres VI

Conference Date: APR 06-10, 2020

Conference Location: ELECTR NETWORK

Conference Sponsors: SPIE, Eurometropole, CNRS, ICube, Univ Strasbourg

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Jasim, Ali A.	I-9646-2014	0000-0003-1606-6322

ISSN: 0277-786X

eISSN: 1996-756X

ISBN: 978-1-5106-3483-1

Record 92 of 236

Title: Primordial mass segregation of star clusters: The role of binary stars

Author(s): Pavlik, V (Pavlik, V)

Source: CONTRIBUTIONS OF THE ASTRONOMICAL OBSERVATORY SKALNATE PLESO Volume: 50 Issue: 2 Pages: 456-460 DOI: 10.31577/caosp.2020.50.2.456 Published: 2020

**Abstract:** Observational results of young star-forming regions suggest that star clusters are completely mass segregated at birth. As a star cluster evolves dynamically, these initial conditions are gradually lost. For star clusters with single stars only and a canonical IMF, it has been suggested that traces of these initial conditions vanish at  $\tau(\nu)$  between 3 and 3.5 half-mass relaxation times. Here, by means of numerical models, we investigate the role of the primordial binary population on the loss of primordial mass segregation. We found that  $\tau(\nu)$  does not depend on the binary star distribution, yielding  $3 < \tau(\nu)/t(\text{rh}) < 3.5$ . We also conclude that the completely mass segregated clusters, even with binaries, are more compatible with the present-day ONC than the non-segregated ones.

Accession Number: WOS:000523574300017

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pavlik, Vaclav C.	8848-2017	0000-0002-3031-062X

ISSN: 1335-1842

eISSN: 1336-0337

Record 93 of 236

Title: Random Phase Approximation Applied to Many-Body Noncovalent Systems

Author(s): Modrzejewski, M (Modrzejewski, Marcin); Yourdkhani, S (Yourdkhani, Sirous); Klimess, J (Klimess, Jfri)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 16 Issue: 1 Pages: 427-442 DOI: 10.1021/acs.jctc.9b00979 Published: JAN 2020

**Abstract:** The random phase approximation (RPA) has received considerable interest in the field of modeling systems where noncovalent interactions are important. Its advantages over widely used density functional theory (DFT) approximations are the exact treatment of exchange and the description of long-range correlation. In this work, we address two open questions related to RPA. First, we demonstrate how accurately RPA describes nonadditive interactions encountered in many-body expansion of a binding energy. We consider three body nonadditive energies in molecular and atomic clusters. Second, we address how the accuracy of RPA depends on input provided by different DFT models, without resorting to self-consistent RPA procedure, which is currently impractical for calculations employing periodic boundary conditions. We find that RPA based on the SCAN0 and PBE0 models, that is, hybrid DFT, achieves an overall accuracy between CCSD and MP3 on a data set of molecular trimers from Rezac et al. (J. Chem. Theory. Comput. 2015, 11, 3065). Finally, many-body expansion for molecular clusters and solids often leads to a large number of small contributions that need to be calculated with high precision. We therefore present a cubic-scaling (or self-consistent field (SCF)-like) implementation of RPA in atomic basis set, which is designed for calculations with high numerical precision.

Accession Number: WOS:000508474800033

PubMed ID: 31738547

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Klimess, Jiri	D-8926-2011	0000-0003-4969-1343
Modrzejewski, Marcin		0000-0001-9979-8355
Yourdkhani, Sirous		0000-0002-7394-6767

ISSN: 1549-9618

eISSN: 1549-9626

Record 94 of 236

Title: Probing the Zr-91 NMR parameters in the solid state by a combination of DFT calculations and experiments

Author(s): Czernek, J (Czernek, Jiri); Kobera, L (Kobera, Libor); Havlak, L (Havlak, Lubomir); Czernekova, V (Czernekova, Vladimira); Rohlicek, J (Rohlicek, Jan); Barta, J (Barta, Jan); Brus, J (Brus, Jiri)

Source: CHEMICAL PHYSICS LETTERS Volume: 738 Article Number: 136855 DOI: 10.1016/j.cplett.2019.136855 Published: JAN 2020

**Abstract:** The practical level of accuracy of the plane-waves (PW) DFT calculations of the Zr-91 chemical shielding (CS) and electric field gradient (EFG) solid-state NMR parameters has been thoroughly investigated to aid in structural studies of crystalline zirconium-containing systems. The CS and EFG data have been shown to be reliably described over wide ranges of benchmarking values by PW DFT calculations with an approximate inclusion of relativistic effects. Based on this, the Zr-91 CS scale has been proposed, and the La2Zr2O7 pyrochlore has been investigated theoretically in terms of spatial orientations of its Zr-91 CS and EFG tensors.

Accession Number: WOS:000501784200042

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Barta, Jan	F-5607-2017	0000-0001-9745-5367
Kobera, Libor	G-5237-2014	0000-0002-8826-948X
Czernek, Jiri	H-6708-2014	
Havlak, Lubomir	G-5743-2014	0000-0002-0160-4522
Brus, Jiri	G-3459-2014	0000-0003-2692-612X
Czernekova, Vladimira		0000-0003-0812-6241
Rohlicek, Jan		0000-0001-6913-2667

ISSN: 0009-2614

eISSN: 1873-4448

Record 95 of 236

Title: Green-, Red-, and Infrared-Emitting Polymorphs of Sterically Hindered Push-Pull Substituted Stilbenes



**Author(s):** Pauk, K (Pauk, Karel); Lunak, S (Lunak, Stanislav, Jr.); Ruzicka, A (Ruzicka, Ales); Markova, A (Markova, Aneta); Mausova, A (Mausova, Anna); Kratochvil, M (Kratochvil, Matous); Melanova, K (Melanova, Klara); Weiter, M (Weiter, Martin); Imramovsky, A (Imramovsky, Ales); Vala, M (Vala, Martin)

**Source:** CHEMISTRY-A EUROPEAN JOURNAL **DOI:** 10.1002/chem.202004419 **Early Access Date:** DEC 2020

**Abstract:** The synthesis, XRD single-crystal structure, powder XRD, and solid-state fluorescence of two new DPA-DPS-EWG derivatives (DPA=diphenylamino, DPS=2,5-diphenyl-stilbene, EWG=electron-withdrawing group, that is, carbaldehyde or dicyanovinylene, DCV) are described. Absorption and fluorescence maxima in solvents of various polarity show bathochromic shifts with respect to the parent DPA-stilbene-EWGs. The electronic coupling in dimers and potential twist elasticity of monomers were studied by density functional theory. Both polymorphs of the CHO derivative emit green fluorescence (527 and 550 nm) of moderate intensity (10 % and 5 %) in polycrystalline powder form. Moderate (5 %) red (672 nm) monomer-like emission was also observed for the first polymorph of the DCV derivative, whereas more intense (32 %) infrared (733 nm) emission of the second polymorph was ascribed to the excimer fluorescence.

**Accession Number:** WOS:000603430700001

**PubMed ID:** 33119919

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Vala, Martin	A-1489-2009	0000-0003-2229-6669

**ISSN:** 0947-6539

**eISSN:** 1521-3765

**Record 96 of 236**

**Title:** Total synthesis of inubosin B

**Author(s):** Hamissa, MF (Hamissa, Mohamed Farouk); Niederhafner, P (Niederhafner, Petr); Safarik, M (Safarik, Martin); Telus, M (Telus, Marta); Kolarova, L (Kolarova, Lenka); Koutna, L (Koutna, Leah); Sestakova, H (Sestakova, Hana); Soucek, R (Soucek, Radko); Sebestik, J (Sebestik, Jaroslav)

**Source:** TETRAHEDRON LETTERS **Volume:** 61 **Issue:** 52 **Article Number:** 152641 **DOI:** 10.1016/j.tetlet.2020.152641 **Published:** DEC 24 2020

**Abstract:** Inubosin B is the most active member of the acridine alkaloids isolated from *Streptomyces* sp. IFM 11440 culture. The inubosins initiate neuroregeneration via a neurogenine 2 pathway. In this work, we have described the total synthesis of inubosin B via two synthetic routes. The effects of various coupling, cyclization and reduction reactions are discussed including common pitfalls and side reactions. Reverse phase chromatography with TFA was crucial for the isolation of the product from aluminum ions present in the reduction media. (C) 2020 Elsevier Ltd. All rights reserved.

**Accession Number:** WOS:000596332600001

**PubMed ID:** 0040-4039

**Record 97 of 236**

**Title:** Transition from Homochiral Clusters to Racemate Monolayers during 2D Crystallization of Trioxa[11]helicene on Ag(100)

**Author(s):** Irziqat, B (Irziqat, Bahaaeddin); Berger, J (Berger, Jan); Mendieta-Moreno, JI (Mendieta-Moreno, Jesus I.); Sundar, MS (Sundar, Mothuku Shyam); Bedekar, AV (Bedekar, Ashutosh V.); Ernst, KH (Ernst, Karl-Heinz)

**Source:** CHEMPHYSICHEM **DOI:** 10.1002/cphc.202000853 **Early Access Date:** DEC 2020

**Abstract:** The phenomenon of chiral crystallization into homochiral crystals is known for more than 170 years, yet it is still poorly understood. Studying crystallization on surfaces under well-defined condition seems a promising approach towards better understanding the intermolecular chiral recognition mechanisms during nucleation and growth. The two-dimensional aggregation of racemic trioxaundecahelicene on the single crystalline silver(100) surface has been investigated with scanning tunneling microscopy and with non-contact atomic force microscopy, as well as molecular modeling simulations. A transition from homochiral cluster motifs to heterochiral assembly into large islands with increasing coverage is observed. Force field modelling confirms higher stability of heterochiral arrangements from twelve molecules on. Results are discussed with respect to previous findings for the all-carbon heptahelicene on the same surface.

**Accession Number:** WOS:000601102500001

**PubMed ID:** 33289221

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Mothuku, Shyam Sundar	AAC-6068-2021	0000-0003-3732-2647
Moreno, Jesus I Mendieta	K-5640-2017	0000-0001-8530-3315

**ISSN:** 1439-4235

**eISSN:** 1439-7641

**Record 98 of 236**

**Title:** Structural Effects of Cation Binding to DPPC Monolayers

**Author(s):** Javanainen, M (Javanainen, Matti); Hua, W (Hua, Wei); Tichacek, O (Tichacek, Ondrej); Delcroix, P (Delcroix, Pauline); Cwiklik, L (Cwiklik, Lukasz); Allen, HC (Allen, Heather C.)

**Source:** LANGMUIR **Volume:** 36 **Issue:** 50 **Pages:** 15258-15269 **DOI:** 10.1021/acs.langmuir.0c02555 **Published:** DEC 22 2020

**Abstract:** Ions at the two sides of the plasma membrane maintain the transmembrane potential, participate in signaling, and affect the properties of the membrane itself. The extracellular leaflet is particularly enriched in phosphatidylcholine lipids and under the influence of Na<sup>+</sup>, Ca<sup>2+</sup>, and Cl<sup>-</sup> ions. In this work, we combined molecular dynamics simulations performed using state-of-the-art models with vibrational sum frequency generation (VSFG) spectroscopy to study the effects of these key ions on the structure of dipalmitoylphosphatidylcholine. We used lipid monolayers as a proxy for membranes, as this approach enabled a direct comparison between simulation and experiment. We find that the effects of Na<sup>+</sup> are minor. Ca<sup>2+</sup>, on the other hand, strongly affects the lipid headgroup conformations and induces a tighter packing of lipids, thus promoting the liquid condensed phase. It does so by binding to both the phosphate and carbonyl oxygens via direct and watermediated binding modes, the ratios of which depend on the monolayer packing. Clustering analysis performed on simulation data revealed that changes in area per lipid or CaCl<sub>2</sub> concentration both affect the headgroup conformations, yet their effects are anticorrelated. Cations at the monolayer surface also attract Cl<sup>-</sup>, which at large CaCl<sub>2</sub> concentrations penetrates deep to the monolayer. This phenomenon coincides with a radical change in the VSFG spectra of the phosphate group, thus indicating the emergence of a new binding mode.

**Accession Number:** WOS:000603297900007

**PubMed ID:** 33296215

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Javanainen, Matti	I-6074-2015	0000-0003-4858-364X
Tichacek, Ondrej	G-5890-2014	0000-0002-3676-8367
Allen, Heather		0000-0003-3120-6784

**ISSN:** 0743-7463

**Record 99 of 236**

**Title:** Platinum(II) Complexes of Tridentate (NN-boolean AND N)-N-boolean AND -Coordinating Ligands Based on Imides, Amides, and Hydrazides: Synthesis and Luminescence Properties

**Author(s):** Puttock, EV (Puttock, Emma, V); Sturala, J (Sturala, Jiri); Kistemaker, JCM (Kistemaker, Jos C. M.); Williams, JAG (Williams, J. A. Gareth)

**Source:** EUROPEAN JOURNAL OF INORGANIC CHEMISTRY **Volume:** 2021 **Issue:** 4 **Pages:** 335-347 **DOI:** 10.1002/ejic.202000879 **Early Access Date:** DEC 2020 **Published:** JAN 26 2021

**Abstract:** Five Pt(II) complexes are described in which the metal ion is bound to anionic (NNN)-N-boolean AND-N-boolean AND-coordinating ligands. The central, deprotonated N atom is derived from an imide Ar-C(=O)-NH-C(=O)-Ar {PtLL-2Cl; Ar=pyridine or pyrimidine}, an amide py-C(=O)-NH-CH<sub>2</sub>-py {(PtLCl)-Cl-3}, or a hydrazide py-C(=O)-NH-N=CH-py {(PtLCl)-Cl-4}. The imide complexes PtLL-2Cl show no significant emission in solution but are modestly bright green/yellow phosphors in the solid state. (PtLCl)-Cl-3 is weakly phosphorescent. (PtLCl)-Cl-4 is formed as a mixture of isomers, bound through either the amido or imino nitrogen, the latter converting to the former upon absorption of light. Remarkably, the imino form displays fluorescence in solution, lambda<sub>max</sub>(0,0)=535 nm, whereas the amido shows phosphorescence, lambda<sub>max</sub>(0,0)=624 nm, tau=440 ns. It is highly unusual for two isomeric compounds to display emission from states of different spin multiplicity. The amido-bound (PtLCl)-Cl-4 can act as a bidentate (ON)-N-boolean AND -coordinating ligand, demonstrated by the formation of bimetallic complexes with iridium(III) or ruthenium(II).

**Accession Number:** WOS:000600778600001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Williams, J A Gareth	F-6618-2012	0000-0002-4688-3000

ISSN: 1434-1948

eISSN: 1099-0682

**Record 100 of 236****Title:** Directionality of light absorption and emission in representative fluorescent proteins**Author(s):** Myskova, J (Myskova, Jitka); Rybakova, O (Rybakova, Olga); Brynda, J (Brynda, Jiri); Khoroshyy, P (Khoroshyy, Petro); Bondar, A (Bondar, Alexey); Lazar, J (Lazar, Josef)**Source:** PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA **Volume:** 117 **Issue:** 51 **Pages:** 32395-32401 **DOI:**10.1073/pnas.2017379117 **Published:** DEC 22 2020**Abstract:** Fluorescent molecules are like antennas: The rate at which they absorb light depends on their orientation with respect to the incoming light wave, and the apparent intensity of their emission depends on their orientation with respect to the observer. However, the directions along which the most important fluorescent molecules in biology, fluorescent proteins (FPs), absorb and emit light are generally not known. Our optical and X-ray investigations of FP crystals have now allowed us to determine the molecular orientations of the excitation and emission transition dipole moments in the FPs mTurquoise2, eGFP, and mCherry, and the photo-convertible FP mEos4b. Our results will allow using FP directionality in studies of molecular and biological processes, but also in development of novel bioengineering and bioelectronics applications.**Accession Number:** WOS:000601315200031**PubMed ID:** 33273123**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Bondar, Alexey	G-9459-2014	0000-0002-1980-2930
Lazar, Josef	H-7487-2014	0000-0002-6285-3995
Bondar, Alexey	AAB-4223-2021	0000-0002-1980-2930
Brynda, Jiri	G-2760-2014	0000-0003-3675-6769

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**Record 101 of 236****Title:** The phylogeny, phylogeography, and diversification history of the westernmost Asian cobra (Serpentes: Elapidae: *Naja oxiana*) in the Trans-Caspian region**Author(s):** Kazemi, E (Kazemi, Elmira); Nazarizadeh, M (Nazarizadeh, Masoud); Fatemizadeh, F (Fatemizadeh, Faezeh); Khani, A (Khani, Ali); Kaboli, M (Kaboli, Mohammad)**Source:** ECOLOGY AND EVOLUTION DOI: 10.1002/ece3.7144 **Early Access Date:** DEC 2020**Abstract:** We conducted a comprehensive analysis of the phylogenetic, phylogeographic, and demographic relationships of Caspian cobra (*Naja oxiana*; Eichwald, 1831) populations based on a concatenated dataset of two mtDNA genes (cyt b and ND4) across the species' range in Iran, Afghanistan, and Turkmenistan, along with other members of Asian cobras (i.e., subgenus *Naja Laurenti*, 1768). Our results robustly supported that the Asiatic *Naja* are monophyletic, as previously suggested by other studies. Furthermore, *N. kaouthia* and *N. sagittifera* were recovered as sister taxa to each other, and in turn sister clades to *N. oxiana*. Our results also highlighted the existence of a single major evolutionary lineage for populations of *N. oxiana* in the Trans-Caspian region, suggesting a rapid expansion of this cobra from eastern to western Asia, coupled with a rapid range expansion from east of Iran toward the northeast. However, across the Iranian range of *N. oxiana*, subdivision of populations was not supported, and thus, a single evolutionary significant unit is proposed for inclusion in future conservation plans in this region.**Accession Number:** WOS:000600661800001**ISSN:** 2045-7758**Record 102 of 236****Title:** Jekyll or Hyde? The genome (and more) of *Nesidiocoris tenuis*, a zoophytophagous predatory bug that is both a biological control agent and a pest**Author(s):** Ferguson, KB (Ferguson, K. B.); Visser, S (Visser, S.); Dalikova, M (Dalikova, M.); Provaznikova, I (Provaznikova, I); Urbaneja, A (Urbaneja, A.); Perez-Hedo, M (Perez-Hedo, M.); Marec, F (Marec, F.); Werren, JH (Werren, J. H.); Zwaan, BJ (Zwaan, B. J.); Pannebakker, BA (Pannebakker, B. A.); Verhulst, EC (Verhulst, E. C.)**Source:** INSECT MOLECULAR BIOLOGY DOI: 10.1111/imb.12688 **Early Access Date:** DEC 2020**Abstract:** *Nesidiocoris tenuis* (Reuter) is an efficient predatory biological control agent used throughout the Mediterranean Basin in tomato crops but regarded as a pest in northern European countries. From the family Miridae, it is an economically important insect yet very little is known in terms of genetic information and no genomic or transcriptomic studies have been published. Here, we use a linked-read sequencing strategy on a single female *N. tenuis*. From this, we assembled the 355 Mbp genome and delivered an ab initio, homology-based and evidence-based annotation. Along the way, the bacterial "contamination" was removed from the assembly. In addition, bacterial lateral gene transfer (LGT) candidates were detected in the *N. tenuis* genome. The complete gene set is composed of 24 688 genes; the associated proteins were compared to other hemipterans (*Cimex lectularis*, *Halyomorpha halys* and *Acyrtosiphon pisum*). We visualized the genome using various cytogenetic techniques, such as karyotyping, CGH and GISH, indicating a karyotype of  $2n = 32$ . Additional analyses include the localization of 18S rDNA and unique satellite probes as well as pooled sequencing to assess nucleotide diversity and neutrality of the commercial population. This is one of the first mirid genomes to be released and the first of a mirid biological control agent.**Accession Number:** WOS:000600782100001**PubMed ID:** 33305885**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Urbaneja, Alberto	C-9071-2011	0000-0001-5986-3685
Dalikova, Martina	J-5722-2015	0000-0002-0266-8894
Marec, Frantisek	G-7943-2014	0000-0002-6745-5603
Ferguson, Kim		0000-0001-6483-1936
Zwaan, Bas	D-8721-2015	0000-0002-8221-4998
Werren, John		0000-0001-9353-2070
Pannebakker, Bart	D-3823-2012	0000-0001-8503-3896

**ISSN:** 0962-1075**eISSN:** 1365-2583**Record 103 of 236****Title:** A diagonalization-free optimization algorithm for solving Kohn-Sham equations of closed-shell molecules**Author(s):** Mrovec, M (Mrovec, Martin); Berger, JA (Berger, J. A.)**Source:** JOURNAL OF COMPUTATIONAL CHEMISTRY DOI: 10.1002/jcc.26472 **Early Access Date:** DEC 2020**Abstract:** A local optimization algorithm for solving the Kohn-Sham equations is presented. It is based on a direct minimization of the energy functional under the equality constraints representing the Grassmann Manifold. The algorithm does not require an eigendecomposition, which may be advantageous in large-scale computations. It is optimized to reduce the number of Kohn-Sham matrix evaluations to one per iteration to be competitive with standard self-consistent field (SCF) approach accelerated by direct inversion of the iterative subspace (DIIS). Numerical experiments include a comparison of the algorithm with DIIS. A high reliability of the algorithm is observed in configurations where SCF iterations fail to converge or find a wrong solution corresponding to a stationary point different from the global minimum. The local optimization algorithm itself does not guarantee that the found minimum is global. However, a randomization of the initial approximation shows a convergence to the right minimum in the vast majority of cases.**Accession Number:** WOS:000600517700001**PubMed ID:** 33347643**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Berger, J.A.	N-2277-2015	0000-0002-4823-520X

**ISSN:** 0192-8651**eISSN:** 1096-987X**Record 104 of 236****Title:** Force Spectroscopy of Iron Tetraphenylporphyrin Molecules with Cl Tips**Author(s):** Scheil, K (Scheil, Katharina); Gruber, M (Gruber, Manuel); Ondracek, M (Ondracek, Martin); Berndt, R (Berndt, Richard)**Source:** JOURNAL OF PHYSICAL CHEMISTRY C Volume: 124 Issue: 49 Pages: 26889-26896 DOI: 10.1021/acs.jpcc.0c08894 **Published:** DEC 10 2020**Abstract:** At low sample voltages, Cl ions may be bidirectionally transferred between a Fe tetraphenylporphyrin (FeTPP) molecule on Au(111) and the tip of a low-temperature scanning tunneling microscope that also operates as an atomic force microscope. Via this effect, Cl-terminated gold tips are prepared. Chlorinated and pristine metal tips are used to probe the forces and conductances of contacts to Au(111), FeTPP, and chlorinated FeTPP. The interaction between the substrate and the Cl ion at the tip may be modeled by a point charge of approximate to -0.3 e interacting with its image. The maximal attraction experienced by the tip in junctions with one Cl ion is much larger when the ion is located at the molecule. Junctions with two Cl ions exhibit two maxima of the attractive force. Simultaneous imaging of the tunneling current and the frequency shift of the force sensor with Cl tips reveals intriguing contrast changes that are tentatively interpreted in terms of tip-induced distortions of the molecules. Density functional theory calculations reproduce important aspects of the experimental data.**Accession Number:** WOS:000599610500037**ISSN:** 1932-7447**eISSN:** 1932-7455**Record 105 of 236****Title:** Interplay between surfactant self-assembly and adsorption at hydrophobic surfaces: insights from dissipative particle dynamics**Author(s):** Sindelka, K (Sindelka, Karel); Lisal, M (Lisal, Martin)**Source:** MOLECULAR PHYSICS Article Number: e1857863 DOI: 10.1080/00268976.2020.1857863 **Early Access Date:** DEC 2020**Abstract:** We study the self-organisation of aqueous surfactants in bulk phase, and the adsorption and self-organisation of the aqueous surfactants at a planar hydrophobic surface by dissipative particle dynamics. Nonionic surfactants, n-alkyl poly(ethylene oxide) CnEm, and water are coarse-grained into mesoscopic beads comprising 1-3 heavy atoms and two water molecules, respectively. The size of the mesoscopic beads is related to the molar volume of the underlying molecular fragments while the bead-bead interaction parameters are calibrated against the water-octanol partition coefficients. We focus on the C6E3, C6E4, C8E3, and C8E4 surfactants in water that form spherical micelles in the bulk. The bulk micellization is primarily affected by the alkyl tail length which is demonstrated by an order of magnitude decrease in the critical micelle concentration when going from the aqueous C6Em to aqueous C8Em solutions. Surfactants strongly adsorb on the hydrophobic surface, adopting lying-down configurations and forming hemispheres which are in equilibrium



with the spherical micelles in the bulk. In contrast to the bulk phase, the surfactant adsorption behaviour is influenced by both the alkyl tail and head chain lengths.

[GRAPHICS]

Accession Number: WOS:000597704100001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sindelka, Karel	E-8790-2014	0000-0003-3925-924X

ISSN: 0026-8976

eISSN: 1362-3028

#### Record 106 of 236

**Title:** Singlet Fission in Thin Solid Films of Bis(thienyl)diketopyrrolopyrroles

**Author(s):** Rais, D (Rais, David); Toman, P (Toman, Petr); Pflieger, J (Pflieger, Jiri); Acharya, U (Acharya, Udit); Panthi, YR (Panthi, Yadu R.); Mensik, M (Mensik, Miroslav); Zhigunov, A (Zhigunov, Alexander); Thottappali, MA (Thottappali, Muhammed A.); Vala, M (Vala, Martin); Markova, A (Markova, Aneta); Stritesky, S (Stritesky, Stanislav); Weiter, M (Weiter, Martin); Ciganeck, M (Ciganeck, Martin); Krajcovic, J (Krajcovic, Jozef); Pauk, K (Pauk, Karel); Imramovsky, A (Imramovsky, Ales); Zaykov, A (Zaykov, Alexandr); Michl, J (Michl, Josef)

**Source:** CHEMPLUSCHEM Volume: 85 Issue: 12 Pages: 2689-2703 DOI: 10.1002/cplu.202000623 Published: DEC 2020

**Abstract:** The singlet fission (SF) process discovered in bis(thienyl)diketopyrrolopyrroles (TDPPs) can boost their potential for photovoltaics (PV). The crystal structures of TDPP analogs carrying n-hexyl, n-butyl, or 2-(adamant-1-yl)ethyl substituents are similar, but contain increasingly slipped stacked neighbor molecules. The observed SF rate constants,  $k(\text{SF})$ , ( $7 \pm 4$ ), ( $9 \pm 3$ ) and ( $5.6 \pm 1.9$ ) ns<sup>-1</sup> for thin films of the three compounds, respectively, are roughly equal, but the triplet quantum yields vary strongly: ( $120 \pm 40$ ), ( $160 \pm 40$ ) and ( $70 \pm 16$ ), respectively. The recent molecular pair model reproduces the near equality of all three  $k(\text{SF})$  at the crystal geometries and identifies all possible pair arrangements in which SF is predicted to be faster, by up to two orders of magnitude. However, it is also clear that the presently non-existent ability to predict the rates of processes competing with SF is pivotal for providing a guide for efforts to optimize the materials for PV.

Accession Number: WOS:000603402700020

PubMed ID: 33332757

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Acharya, Udit	B-7149-2018	0000-0001-9761-0785
Michl, Josef	G-9376-2014	
Thottappali, Muhammed Arshad	AAA-8403-2021	

ISSN: 2192-6506

#### Record 107 of 236

**Title:** A Cross-Domain Comparative Study of Big Data Architectures

**Author(s):** Macak, M (Macak, Martin); Ge, MZ (Ge, Mouzhi); Buhnova, B (Buhnova, Barbora)

**Source:** INTERNATIONAL JOURNAL OF COOPERATIVE INFORMATION SYSTEMS Volume: 29 Issue: 4 Article Number: 2030001 DOI: 10.1142/S0218843020300016 Published: DEC 2020

**Abstract:** Nowadays, a variety of Big Data architectures are emerging to organize the Big Data life cycle. While some of these architectures are proposed for general usage, many of them are proposed in a specific application domain such as smart cities, transportation, healthcare, and agriculture. There is, however, a lack of understanding of how and why Big Data architectures vary in different domains and how the Big Data architecture strategy in one domain may possibly advance other domains. Therefore, this paper surveys and compares the Big Data architectures in different application domains. It also chooses a representative architecture of each researched application domain to indicate which Big Data architecture from a given domain the researchers and practitioners may possibly start from. Next, a pairwise cross-domain comparison among the Big Data architectures is presented to outline the similarities and differences between the domain-specific architectures. Finally, the paper provides a set of practical guidelines for Big Data researchers and practitioners to build and improve Big Data architectures based on the knowledge gathered in this study.

Accession Number: WOS:000603594000001

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eISSN: 1793-6365

#### Record 108 of 236

**Title:** Semantic Segmentation of Intralobular and Extralobular Tissue from Liver Scaffold H&E Images

**Author(s):** Jirik, M (Jirik, Miroslav); Gruber, I (Gruber, Ivan); Moulisova, V (Moulisova, Vladimira); Schindler, C (Schindler, Claudia); Cervenkova, L (Cervenkova, Lenka); Palek, R (Palek, Richard); Rosendorf, J (Rosendorf, Jachym); Arlt, J (Arlt, Janine); Bolek, L (Bolek, Lukas); Dejmek, J (Dejmek, Jiri); Dahmen, U (Dahmen, Uta); Zelezny, M (Zelezny, Milos); Liska, V (Liska, Vaclav)

**Source:** SENSORS Volume: 20 Issue: 24 Article Number: 7063 DOI: 10.3390/s20247063 Published: DEC 2020

**Abstract:** Decellularized tissue is an important source for biological tissue engineering. Evaluation of the quality of decellularized tissue is performed using scanned images of hematoxylin-eosin stained (H&E) tissue sections and is usually dependent on the observer. The first step in creating a tool for the assessment of the quality of the liver scaffold without observer bias is the automatic segmentation of the whole slide image into three classes: the background, intralobular area, and extralobular area. Such segmentation enables to perform the texture analysis in the intralobular area of the liver scaffold, which is crucial part in the recellularization procedure. Existing semi-automatic methods for general segmentation (i.e., thresholding, watershed, etc.) do not meet the quality requirements. Moreover, there are no methods available to solve this task automatically. Given the low amount of training data, we proposed a two-stage method. The first stage is based on classification of simple hand-crafted descriptors of the pixels and their neighborhoods. This method is trained on partially annotated data. Its outputs are used for training of the second-stage approach, which is based on a convolutional neural network (CNN). Our architecture inspired by U-Net reaches very promising results, despite a very low amount of the training data. We provide qualitative and quantitative data for both stages. With the best training setup, we reach 90.70% recognition accuracy.

Accession Number: WOS:000603179000001

PubMed ID: 33321713

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Gruber, Ivan		0000-0003-2333-433X
Rosendorf, Jachym		0000-0003-2125-0685
Jirik, Miroslav	S-4251-2017	0000-0002-8002-2079

eISSN: 1424-8220

#### Record 109 of 236

**Title:** Bruton's Tyrosine Kinase Inhibitors Ibrutinib and Acalabrutinib Counteract Anthracycline Resistance in Cancer Cells Expressing AKR1C3

**Author(s):** Morell, A (Morell, Anselm); Cermakova, L (Cermakova, Lucie); Novotna, E (Novotna, Eva); Lastovickova, L (Lastovickova, Lenka); Haddad, M (Haddad, Melodie); Haddad, A (Haddad, Andrew); Portillo, R (Portillo, Ramon); Wsol, V (Wsol, Vladimir)

**Source:** CANCERS Volume: 12 Issue: 12 Article Number: 3731 DOI: 10.3390/cancers12123731 Published: DEC 2020

**Abstract:** Simple Summary

The enzyme aldo-keto reductase 1C3 (AKR1C3) is present in several cancers, in which it is capable of actively metabolising different chemotherapy drugs and decreasing their cytotoxic effects. Therefore, the combination with specific inhibitors of AKR1C3 might prevent drug metabolism and increase its efficacy. We investigated the ability of Bruton's tyrosine kinase inhibitors ibrutinib and acalabrutinib to block the AKR1C3 mediated inactivation of the anthracycline daunorubicin. Experimentation with recombinant AKR1C3 and different cancer cells expressing this enzyme outlined BTK-inhibitors as potential partners to synergise daunorubicin cytotoxicity in vitro. This evidence could be useful to improve the clinical outcome of anthracycline-based chemotherapies.

Over the last few years, aldo-keto reductase family 1 member C3 (AKR1C3) has been associated with the emergence of multidrug resistance (MDR), thereby hindering chemotherapy against cancer. In particular, impaired efficacy of the gold standards of induction therapy in acute myeloid leukaemia (AML) has been correlated with AKR1C3 expression, as this enzyme metabolises several drugs including anthracyclines. Therefore, the development of selective AKR1C3 inhibitors may help to overcome chemoresistance in clinical practice. In this regard, we demonstrated that Bruton's tyrosine kinase (BTK) inhibitors ibrutinib and acalabrutinib efficiently prevented daunorubicin (Dau) inactivation mediated by AKR1C3 in both its recombinant form as well as during its overexpression in cancer cells. This revealed a synergistic effect of BTK inhibitors on Dau cytotoxicity in cancer cells expressing AKR1C3 both exogenously and endogenously, thus reverting anthracycline resistance in vitro. These findings suggest that BTK inhibitors have a novel off-target action, which can be exploited against leukaemia through combination regimens with standard chemotherapeutics like anthracyclines.

Accession Number: WOS:000601803400001

PubMed ID: 33322571

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Cermakova, Lucie		0000-0002-2322-4096
Wsol, Vladimir	K-3476-2016	0000-0003-3745-7648

eISSN: 2072-6694

**Record 110 of 236****Title:** Prediction of pKa in a system with high orthogonal barriers: Alchemical flying Gaussian method**Author(s):** Trapl, D (Trapl, Dalibor); del Rio, CC (del Rio, Carmen Cuerdo); Kriz, P (Kriz, Pavel); Spiwok, V (Spiwok, Vojtech)**Source:** CHEMICAL PHYSICS LETTERS Volume: 760 Article Number: 138012 DOI: 10.1016/j.cplett.2020.138012 Published: DEC 2020

**Abstract:** Alchemical simulations are versatile tools for prediction of relative free energy differences. The accuracy of these methods depends critically on sampling of orthogonal (non-alchemical) degrees of freedom. Here we apply the flying Gaussian method to accelerate orthogonal degrees of freedom in peptide bond cis/trans isomerisation. The approach is demonstrated on prediction of pKa value of N-acetylproline. Isomerization of the amide bond was accelerated in this simulation by multiple orders of magnitude. Alchemical free energy was obtained by reweighting. The results show that a combination of alchemical and flying Gaussian simulations is suitable for systems with high (similar to 60 kJ/mol) energy barrier.

Accession Number: WOS:000596603000008

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Trapl, Dalibor		0000-0002-3435-5841

ISSN: 0009-2614

eISSN: 1873-4448

**Record 111 of 236****Title:** Anomalous Freezing of Low-Dimensional Water Confined in Graphene Nanowrinkles**Author(s):** Verhagen, T (Verhagen, Tim); Klimes, J (Klimes, Jiri); Pacakova, B (Pacakova, Barbara); Kalbac, M (Kalbac, Martin); Vejpravova, J (Vejpravova, Jana)**Source:** ACS NANO Volume: 14 Issue: 11 Pages: 15587-15594 DOI: 10.1021/acsnano.0c03161 Published: NOV 24 2020

**Abstract:** Various properties of water are affected by confinement as the space-filling of the water molecules is very different from bulk water. In our study, we challenged the creation of a stable system in which water molecules are permanently locked in nanodimensional graphene traps. For that purpose, we developed a technique, nitrocellulose-assisted transfer of graphene grown by chemical vapor deposition, which enables capturing of the water molecules below an atomically thin graphene membrane structured into a net of regular wrinkles with a lateral dimension of about 4 nm. After successfully confining water molecules below a graphene monolayer, we employed cryogenic Raman spectroscopy to monitor the phase changes of the confined water as a function of the temperature. In our experiment system, the graphene monolayer structured into a net of fine wrinkles plays a dual role: (i) it enables water confinement and (ii) serves as an extremely sensitive probe for phase transitions involving water via graphene-based spectroscopic monitoring of the underlying water structure. Experimental findings were supported with classical and path integral molecular dynamics simulations carried out on our experimental system. Results of simulations show that surface premelting of the ice confined within the wrinkles starts at similar to 200 K and the melting process is complete at similar to 240 K, which is far below the melting temperature of bulk water ice. The processes correspond to changes in the doping and strain in the graphene tracked by Raman spectroscopy. We conclude that water can be confined between graphene structured into nanowrinkles and silica substrate and its phase transitions can be tracked via Raman spectral feature of the encapsulating graphene. Our study also demonstrated that peculiar behavior of liquids under spatial confinement can be inspected via the optical response of atomically thin graphene sensors.

Accession Number: WOS:000595533800101

PubMed ID: 33119250

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Verhagen, Tim		0000-0001-7703-221X
Vejpravova, Jana	G-1895-2014	0000-0002-6308-9992

ISSN: 1936-0851

eISSN: 1936-086X

**Record 112 of 236****Title:** Perturbative and nonperturbative photoionization of H-2 and H2O using the molecular R-matrix-with-time method**Author(s):** Benda, J (Benda, J.); Gorfinkiel, JD (Gorfinkiel, J. D.); Masin, Z (Masin, Z.); Armstrong, GSJ (Armstrong, G. S. J.); Brown, AC (Brown, A. C.); Clarke, DDA (Clarke, D. D. A.); van der Hart, HW (van der Hart, H. W.); Wragg, J (Wragg, J.)**Source:** PHYSICAL REVIEW A Volume: 102 Issue: 5 Article Number: 052826 DOI: 10.1103/PhysRevA.102.052826 Published: NOV 23 2020

**Abstract:** The ab initio R-matrix with time method has recently been extended to allow simulation of fully nonperturbative multielectron processes in molecules driven by ultrashort arbitrarily polarized strong laser fields. Here we demonstrate the accuracy and capabilities of the current implementation of the method for two targets: We study single-photon and multiphoton ionization of H-2 and one-photon and strong-field ionization of H2O and compare the results to available experimental and theoretical data as well as our own time-independent R-matrix calculations. We obtain a highly accurate description of total and state-to-state single-photon ionization of H2O and, using a simplified coupled-channel model, we show that state coupling is essential to obtain qualitatively correct results and that its importance as a function of laser intensity changes. We find that electron correlation plays a more important role at low intensities (up to approximately 50 TW/cm(2)).

Accession Number: WOS:000591727600010

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Benda, Jakub	G-3302-2010	0000-0003-0965-2040
Armstrong, Gregory	AAO-2580-2020	0000-0001-5949-2626
Brown, Andrew C	C-2692-2013	0000-0001-5652-1495
Gorfinkiel, Jimena		0000-0001-9264-3932

ISSN: 2469-9926

eISSN: 2469-9934

**Record 113 of 236****Title:** Polymorphism of Amyloid Fibrils Induced by Catalytic Seeding: A Vibrational Circular Dichroism Study**Author(s):** Krupova, M (Krupova, Monika); Kessler, J (Kessler, Jiri); Bour, P (Bour, Petr)**Source:** CHEMPHYSICHEM Volume: 22 Issue: 1 Pages: 83-91 DOI: 10.1002/cphc.202000797 Early Access Date: NOV 2020 Published: JAN 7 2021

**Abstract:** Amyloid protein fibrils occur in many biological events, but their formation and structural variability are understood rather poorly. We systematically explore fibril polymorphism for polyglutamic acid (PGA), insulin and hen egg white lysozyme. The fibrils were grown in the presence of "seeds", that is fibrils of the same or different protein. The seeds in concentrations higher than about 5 % of the total protein amount fully determined the structure of the final fibrils. Fibril structure was monitored by vibrational circular dichroism (VCD) spectroscopy and other techniques. The VCD shapes significantly differ for different fibril samples. Infrared (IR) and VCD spectra of PGA were also simulated using density functional theory (DFT) and a periodic model. The simulation provides excellent basis for data interpretation and reveals that the spectral shapes and signs depend both on fibril length and twist. The understanding of fibril formation and interactions may facilitate medical treatment of protein misfolding diseases in the future.

Accession Number: WOS:000591515600001

PubMed ID: 33080105

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Krupova, Monika T-1224-2017 0000-0002-5994-4247

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**Record 114 of 236****Title:** Curie-Weiss susceptibility in strongly correlated electron systems**Author(s):** Janis, V (Janis, Vaclav); Klic, A (Klic, Antonin); Yan, JW (Yan, Jiawei); Pokorny, V (Pokorny, Vladislav)**Source:** PHYSICAL REVIEW B **Volume:** 102 **Issue:** 20 **Article Number:** 205120 **DOI:** 10.1103/PhysRevB.102.205120 **Published:** NOV 19 2020**Abstract:** The genesis of the Curie-Weiss magnetic response observed in most transition metals that are Fermi liquids at low temperatures has been an enigma for decades and has not yet been fully explained from microscopic principles. We show on the single-impurity Anderson model how the quantum dynamics of strong electron correlations leads to the Curie-Weiss magnetic susceptibility sufficiently above the Kondo temperature. Such behavior has not yet been demonstrated and can be observed only when the bare interaction is substantially screened (renormalized) and a balance between quantum and thermal fluctuations is kept. We set quantitative criteria for the existence of the Curie-Weiss law.**Accession Number:** WOS:000590408200004**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pokorny, Vladislav	G-5750-2014	0000-0002-8944-6417
Janis, Vaclav	A-8379-2011	0000-0001-5959-6935

ISSN: 2469-9950

eISSN: 2469-9969

**Record 115 of 236****Title:** Monitoring peptide tyrosine nitration by spectroscopic methods**Author(s):** Niederhafner, P (Niederhafner, Petr); Safarik, M (Safarik, Martin); Neburkova, J (Neburkova, Jitka); Keiderling, TA (Keiderling, Timothy A.); Bour, P (Bour, Petr); Sebestik, J (Sebestik, Jaroslav)**Source:** AMINO ACIDS **DOI:** 10.1007/s00726-020-02911-7 **Early Access Date:** NOV 2020**Abstract:** Oxidative stress can lead to various derivatives of the tyrosine residue in peptides and proteins. A typical product is 3-nitro-L-tyrosine residue (Nit), which can affect protein behavior during neurodegenerative processes, such as those associated with Alzheimer's and Parkinson's diseases. Surface enhanced Raman spectroscopy (SERS) is a technique with potential for detecting peptides and their metabolic products at very low concentrations. To explore the applicability to Nit, we use SERS to monitor tyrosine nitration in Met-enkephalin, rev-Prion protein, and alpha-synuclein models. Useful nitration indicators were the intensity ratio of two tyrosine marker bands at 825 and 870 cm<sup>-1</sup> and a bending vibration of the nitro group. During the SERS measurement, a conversion of nitrotyrosine to azobenzene containing peptides was observed. The interpretation of the spectra has been based on density functional theory (DFT) simulations. The CAM-B3LYP and omega B97XD functionals were found to be most suitable for modeling the measured data. The secondary structure of the alpha-synuclein models was monitored by electronic and vibrational circular dichroism (ECD and VCD) spectroscopies and modeled by molecular dynamics (MD) simulations. The results suggest that the nitration in these peptides has a limited effect on the secondary structure, but may trigger their aggregation.**Accession Number:** WOS:000590203400001**PubMed ID:** 33205301**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Sebestik, Jaroslav	C-9166-2012	0000-0002-0614-2064

ISSN: 0939-4451

eISSN: 1438-2199

**Record 116 of 236****Title:** A new species of *Pristimantis* (Amphibia, Anura, Strabomantidae) from the Pui Pui Protected Forest (central Peru), with comments on *Pristimantis albertus* Duellman & Hedges, 2007**Author(s):** Moravec, J (Moravec, Jiri); Lehr, E (Lehr, Edgar); Kodejs, K (Kodejs, Karel)**Source:** ZOOKEYS **Issue:** 994 **Pages:** 125-148 **DOI:** 10.3897/zookeys.994.56277 **Published:** NOV 17 2020**Abstract:** We describe a new *Pristimantis* species from the eastern Andes, Region Junin, Peru following an integrative taxonomic approach. The description is based on three adult males (snout-vent length 25.7-28.8 mm) collected in two montane forests between 1615 and 1800 m a.s.l. in the Pui Pui Protected Forest and its close surroundings. The new species is mainly characterised by absence of tympanum, presence of inner tarsal fold, broad horizontal red band across iris, ventre mottled black and cream and ventral surfaces of thighs salmon and grey mottled. Amongst the Amazonian and montane forest *Pristimantis* that have the ventre and groin contrastingly black and cream mottled, *P. sinschi* sp. nov. is morphologically most similar to *P. lindae* and *P. ventrimarmoratus*. However, DNA barcoding revealed a clear distinction between these three species and placed *P. sinschi* sp. nov. as sister taxon of *P. lindae*. We designate a lectotype for *P. ventrimarmoratus* and restrict the type locality of this species to "El Topo, R. Pastaza, [Provincia Tungurahua,] E. Ecuador, 4200 feet". *Pristimantis albertus* and *P. sagittulus* are recorded for the first time in the Region Junin. Additional data on morphology and systematics are provided for *P. albertus*.**Accession Number:** WOS:000590769600002**PubMed ID:** 33273884

ISSN: 1313-2989

eISSN: 1313-2970

**Record 117 of 236****Title:** Fundamental gap of fluorographene by many-body GW and fixed-node diffusion Monte Carlo methods**Author(s):** Dubecky, M (Dubecky, Matus); Karlicky, F (Karlicky, Frantisek); Minarik, S (Minarik, Stanislav); Mitas, L (Mitas, Lubos)**Source:** JOURNAL OF CHEMICAL PHYSICS **Volume:** 153 **Issue:** 18 **Article Number:** 184706 **DOI:** 10.1063/5.0030952 **Published:** NOV 14 2020**Abstract:** Fluorographene (FG) is a promising graphene-derived material with a large bandgap. Currently existing predictions of its fundamental gap ( $\Delta$ ) and optical gap ( $\Delta_{opt}$ ) significantly vary when compared with experiment. We provide here an ultimate benchmark of  $\Delta$  for FG by many-body GW and fixed-node diffusion Monte Carlo (FNDMC) methods. Both approaches independently arrive at  $\Delta$  approximate to 7.1 +/- 0.1 eV. In addition, the Bethe-Salpeter equation enabled us to determine the first exciton binding energy,  $E_b = 1.92$  eV. We also point to the possible misinterpretation problem of the results obtained for gaps of solids by FNDMC with single-reference trial wave functions of Bloch orbitals. We argue why instead of  $\Delta_{opt}$ , in the thermodynamic limit, such an approach results in energy differences that rather correspond to  $\Delta$ , and we also outline conditions when this case actually applies.**Accession Number:** WOS:000593964100001**PubMed ID:** 33187427**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Karlicky, Frantisek	E-8067-2010	0000-0002-2623-3991

ISSN: 0021-9606

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**Record 118 of 236****Title:** Ring-closing metathesis of prochiral oxanediynes to racemic 4-alkenyl-2-alkynyl-3,6-dihydro-2H-pyrans**Author(s):** Kolarikova, V (Kolarikova, Viola); Rybackova, M (Rybackova, Marketa); Svoboda, M (Svoboda, Martin); Kvicala, J (Kvicala, Jaroslav)**Source:** BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY **Volume:** 16 **Pages:** 2757-2768 **DOI:** 10.3762/bjoc.16.226 **Published:** NOV 13 2020**Abstract:** The prochiral 4-(allyloxy)hepta-1,6-dienes, optionally modified in the positions 1 and 7 with an alkyl or ester group, undergo a chemoselective ring-closing enyne metathesis yielding racemic 4-alkenyl-2-alkynyl-3,6-dihydro-2H-pyrans. Among the catalysts tested, Grubbs 1st generation precatalyst in the presence of ethene (Mori conditions) gave superior results compared to the more stable Grubbs or Hoveyda-Grubbs 2nd generation precatalysts. This is probably caused by a suppression of the subsequent side-reactions of the enyne metathesis product with ethene. On the other hand, the 2nd generation precatalysts gave better yields in the absence of ethene. The metathesis products, containing both a triple bond and a conjugated system, can be successfully orthogonally modified. For example, the metathesis product of 5-(allyloxy)nona-2,7-diyne reacted chemo- and stereoselectively in a Diels-Alder reaction with N-phenylmaleimide affording the tricyclic products as a mixture of two separable diastereoisomers, the configuration of which was estimated by DFT



computations. The reported enediyne metathesis paves the way to the enantioselective enyne metathesis yielding chiral building blocks for compounds with potential biological activity, e.g., norsalvinorin or cacospongionolide B.

**Accession Number:** WOS:000591079700001

**PubMed ID:** 33224302

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kvicala, Jaroslav		0000-0002-9713-021X

ISSN: 1860-5397

#### Record 119 of 236

**Title:** Benchmark Data Sets of Boron Cluster Dihydrogen Bonding for the Validation of Approximate Computational Methods

**Author(s):** Fanfrlik, J (Fanfrlik, Jindrich); Pecina, A (Pecina, Adam); Rezac, J (Rezac, Jan); Lepsik, M (Lepsik, Martin); Sarosi, MB (Sarosi, Menyhart B.); Hnyk, D (Hnyk, Drahomir); Hobza, P (Hobza, Pavel)

**Source:** CHEMPHYSCHEM Volume: 21 Issue: 23 Pages: 2599-2604 DOI: 10.1002/cphc.202000729 Early Access Date: NOV 2020 Published: DEC 2 2020

**Abstract:** The success of approximate computational methods, such as molecular mechanics, or dispersion-corrected density functional theory, in the description of non-covalent interactions relies on accurate parameterizations. Benchmark data sets are thus required. This area is well developed for organic molecules and biomolecules but practically non-existent for boron clusters, which have been gaining in importance in modern drug as well as material design. To fill this gap, we have introduced two data sets featuring the most common non-covalent interaction of boron clusters, the dihydrogen bond, and calculated reference interaction energies at the "golden standard" CCSD(T)/CBS level. The boron clusters studied interact with formamide, methanol, water and methane at various distances and in two geometrical arrangements. The performance of the tested approximate methods is variable and recommendations for further use are given.

**Accession Number:** WOS:000588417900001

**PubMed ID:** 33179424

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Rezac, Jan	A-9107-2010	0000-0001-6849-7314
Pecina, Adam	K-2304-2012	0000-0003-3890-7831
Lepsik, Martin	C-6614-2012	0000-0003-2607-8132
Fanfrlik, Jindrich		0000-0002-1257-1201

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#### Record 120 of 236

**Title:** One- and two-point source statistics from the LOFAR Two-metre Sky Survey first data release

**Author(s):** Siewert, TM (Siewert, T. M.); Hale, C (Hale, C.); Bhardwaj, N (Bhardwaj, N.); Biermann, M (Biermann, M.); Bacon, DJ (Bacon, D. J.); Jarvis, M (Jarvis, M.); Rottgering, HJA (Rottgering, H. J. A.); Schwarz, DJ (Schwarz, D. J.); Shimwell, T (Shimwell, T.); Best, PN (Best, P. N.); Duncan, KJ (Duncan, K. J.); Hardcastle, MJ (Hardcastle, M. J.); Sabater, J (Sabater, J.); Tasse, C (Tasse, C.); White, GJ (White, G. J.); Williams, WL (Williams, W. L.)

**Source:** ASTRONOMY & ASTROPHYSICS Volume: 643 Article Number: A100 DOI: 10.1051/0004-6361/201936592 Published: NOV 10 2020

**Abstract:** Context. The LOFAR Two-metre Sky Survey (LoTSS) will eventually map the complete Northern sky and provide an excellent opportunity to study the distribution and evolution of the large-scale structure of the Universe. Aims. We test the quality of LoTSS observations through a statistical comparison of the LoTSS first data release (DR1) catalogues to expectations from the established cosmological model of a statistically isotropic and homogeneous Universe. Methods. We study the point-source completeness and define several quality cuts, in order to determine the count-in-cell statistics and differential source count statistics, and measure the angular two-point correlation function. We use the photometric redshift estimates, which are available for about half of the LoTSS-DR1 radio sources, to compare the clustering throughout the history of the Universe. Results. For the masked LoTSS-DR1 value-added source catalogue, we find a point-source completeness of 99% above flux densities of 0.8 mJy. The counts-in-cell statistic reveals that the distribution of radio sources cannot be described by a spatial Poisson process. Instead, a good fit is provided by a compound Poisson distribution. The differential source counts are in good agreement with previous findings in deep fields at low radio frequencies and with simulated catalogues from the SKA Design Study and the Tiered Radio Extragalactic Continuum Simulation. Restricting the value added source catalogue to low-noise regions and applying a flux density threshold of 2 mJy provides our most reliable estimate of the angular two-point correlation. Based on the distribution of photometric redshifts and the Planck 2018 best-fit cosmological model, the theoretically predicted angular two-point correlation between 0.1 deg and 6 deg agrees reasonably well with the measured clustering for the sub-sample of radio sources with redshift information. Conclusions. The deviation from a Poissonian distribution might be a consequence of the multi-component nature of a large number of resolved radio sources and/or of uncertainties on the flux density calibration. The angular two-point correlation function is  $< 10^{-2}$  at angular scales  $> 1$  deg and up to the largest scales probed. At a 2 mJy flux density threshold and at a pivot angle of 1 deg, we find a clustering amplitude of  $A = (5.1 \pm 0.6) \times 10^{-3}$  with a slope parameter of  $\gamma = 0.74 \pm 0.16$ . For smaller flux density thresholds, systematic issues are identified, which are most likely related to the flux density calibration of the individual pointings. We conclude that we find agreement with the expectation of large-scale statistical isotropy of the radio sky at the per cent level. The angular two-point correlation agrees well with the expectation of the cosmological standard model.

**Accession Number:** WOS:000594764600001

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#### Record 121 of 236

**Title:** Decoding the intricate network of molecular interactions of a hyperstable engineered biocatalyst

**Author(s):** Markova, K (Markova, Klara); Chmelova, K (Chmelova, Klaudia); Marques, SM (Marques, Sergio M.); Carpentier, P (Carpentier, Philippe); Bednar, D (Bednar, David); Damborsky, J (Damborsky, Jiri); Marek, M (Marek, Martin)

**Source:** CHEMICAL SCIENCE Volume: 11 Issue: 41 Pages: 11162-11178 DOI: 10.1039/d0sc03367g Published: NOV 7 2020

**Abstract:** Computational design of protein catalysts with enhanced stabilities for use in research and enzyme technologies is a challenging task. Using force-field calculations and phylogenetic analysis, we previously designed the haloalkane dehalogenase DhaA115 which contains 11 mutations that confer upon it outstanding thermostability ( $T_m = 73.5$  degrees C;  $\Delta T_m > 23$  degrees C). An understanding of the structural basis of this hyperstabilization is required in order to develop computer algorithms and predictive tools. Here, we report X-ray structures of DhaA115 at 1.55 angstrom and 1.6 angstrom resolutions and their molecular dynamics trajectories, which unravel the intricate network of interactions that reinforce the  $\alpha$ -sandwich architecture. Unexpectedly, mutations toward bulky aromatic amino acids at the protein surface triggered long-distance (similar to 27 angstrom) backbone changes due to cooperative effects. These cooperative interactions produced an unprecedented double-lock system that: (i) induced backbone changes, (ii) closed the molecular gates to the active site, (iii) reduced the volumes of the main and slot access tunnels, and (iv) occluded the active site. Despite these spatial restrictions, experimental tracing of the access tunnels using krypton derivative crystals demonstrates that transport of ligands is still effective. Our findings highlight key thermostabilization effects and provide a structural basis for designing new thermostable protein catalysts.

**Accession Number:** WOS:000582936200030

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Bednar, David	ABF-5943-2020	0000-0002-6803-0340
Marques, Sergio M	H-8685-2012	0000-0002-6281-7505
Damborsky, Jiri	H-3799-2012	0000-0002-7848-8216

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#### Record 122 of 236

**Title:** 1D Coordination pi-d Conjugated Polymers with Distinct Structures Defined by the Choice of the Transition Metal: Towards a New Class of Antiaromatic Macrocycles

**Author(s):** Santhini, VM (Santhini, Vijai M.); Wackerlin, C (Wackerlin, Christian); Cahlik, A (Cahlik, Ales); Ondracek, M (Ondracek, Martin); Pascal, S (Pascal, Simon); Matej, A (Matej, Adam); Stetsovych, O (Stetsovych, Oleksandr); Mutombo, P (Mutombo, Pingo); Lazar, P (Lazar, Petr); Siri, O (Siri, Olivier); Jelinek, P (Jelinek, Pavel)

**Source:** ANGEWANDTE CHEMIE-INTERNATIONAL EDITION Volume: 60 Issue: 1 Pages: 439-445 DOI: 10.1002/anie.202011462 Early Access Date: NOV 2020 Published: JAN 4 2021

**Abstract:** Recently pi-d conjugated coordination polymers have received a lot of attention owing to their unique material properties, although synthesis of long and defect-free polymers remains challenging. Herein we introduce a novel on-surface synthesis of coordination polymers with quinoidal ligands under ultra-high vacuum conditions, which enables formation of flexible coordination polymers with lengths up to hundreds of nanometers. Moreover, this procedure allows the incorporation of different transition-metal atoms with four- or two-fold coordination. Remarkably, the two-fold coordination mode revealed the formation of wires constituted by (electronically) independent 12-membered antiaromatic macrocycles linked together through two C-C single bonds.

**Accession Number:** WOS:000584114800001

**PubMed ID:** 32886405

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pascal, Simon	J-7140-2018	0000-0001-8387-494X
Wackerlin, Christian	C-7612-2018	0000-0001-6587-1235
Lazar, Petr	C-1074-2011	0000-0002-7312-3656
Jelinek, Pavel	ABE-8589-2020	0000-0002-5645-8542
SIRI, Olivier	ABC-8735-2020	0000-0001-9747-3813
Wackerlin, Christian	AAC-9097-2021	0000-0001-6587-1235
Mutombo, Pingo	G-5266-2014	0000-0002-8175-7587
Stetsovych, Oleksandr		0000-0001-7788-1617

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**Record 123 of 236**

**Title:** Enhanced DNA damage response through RAD50 in triple negative breast cancer resistant and cancer stem-like cells contributes to chemoresistance

**Author(s):** Abad, E (Abad, Etna); Civit, L (Civit, Laia); Potesil, D (Potesil, David); Zdrahal, Z (Zdrahal, Zbynek); Lyakhovich, A (Lyakhovich, Alex)

**Source:** FEBS JOURNAL **DOI:** 10.1111/febs.15588 **Early Access Date:** NOV 2020

**Abstract:** A growing body of evidence supports the notion that cancer resistance is driven by a small subset of cancer stem cells (CSC), responsible for tumor initiation, growth, and metastasis. Both CSC and chemoresistant cancer cells may share common qualities to activate a series of self-defense mechanisms against chemotherapeutic drugs. Here, we aimed to identify proteins in chemoresistant triple-negative breast cancer (TNBC) cells and corresponding CSC-like spheroid cells that may contribute to their resistance. We have identified several candidate proteins representing the subfamilies of DNA damage response (DDR) system, the ATP-binding cassette, and the 26S proteasome degradation machinery. We have also demonstrated that both cell types exhibit enhanced DDR when compared to corresponding parental counterparts, and identified RAD50 as one of the major contributors in the resistance phenotype. Finally, we have provided evidence that depleting or blocking RAD50 within the Mre11-Rad50-NBS1 (MRN) complex resensitizes CSC and chemoresistant TNBC cells to chemotherapeutic drugs.

**Accession Number:** WOS:000584017500001

**PubMed ID:** 33090711

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lyakhovich, Alex	B-4410-2008	0000-0002-8279-4697
ABAD, ETNA		0000-0002-9431-5817

**ISSN:** 1742-464X

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**Record 124 of 236**

**Title:** Unexpected cryptic species diversity of parasites of the family Xenidae (Strepsiptera) with a constant diversification rate over time

**Author(s):** Benda, D (Benda, Daniel); Votykova, K (Votykova, Katerina); Nakase, Y (Nakase, Yuta); Straka, J (Straka, Jakub)

**Source:** SYSTEMATIC ENTOMOLOGY **Volume:** 46 **Issue:** 1 **Pages:** 252-265 **DOI:** 10.1111/syen.12460 **Early Access Date:** NOV 2020 **Published:** JAN 2021

**Abstract:** Parasitism is one of the most successful and ancient strategies. Due to the specialized lifestyle of parasites, they are usually affected by reductions and changes in their body plan in comparison with nonparasitic sister groups. Extreme environmental conditions may impose restraints on behavioural or physiological adaptations to a specific host and limit morphological changes associated with speciation. Such morphological homogeneity has led to the diversity of parasites being underestimated in morphological studies. By contrast, the species concept has dramatically changed in many parasitic groups during recent decades of study using DNA sequence data. Here we tested the phenomenon of cryptic species diversity in the twisted-wing parasite family Xenidae (Strepsiptera) using nuclear and mitochondrial DNA sequence data for a broad sample of Xenidae. We used three quantitative methods of species delimitation from the molecular phylogenetic data - one distance-based (ABGD) and two tree-based (GMYC, bPTP). We found 77-96 putative species in our data and suggested the number of Xenidae species to be more diverse than expected. We identified 67 hosts to species level and almost half of them were not previously known as hosts of Xenidae. The mean number of host species per putative species varied between 1.39 and 1.55. The constant rate in net diversification can be explained by the flexibility of this parasitic group, represented by their ability to colonize new host lineages combined with passive long-range dispersal by hosts.

**Accession Number:** WOS:000584104400001

**ISSN:** 0307-6970

**eISSN:** 1365-3113

**Record 125 of 236**

**Title:** Fast magnetic field amplification in distant galaxy clusters

**Author(s):** Di Gennaro, G (Di Gennaro, Gabriella); van Weeren, RJ (van Weeren, Reinout J.); Brunetti, G (Brunetti, Gianfranco); Cassano, R (Cassano, Rossella); Bruggen, M (Brueggen, Marcus); Hoeft, M (Hoeft, Matthias); Shimwell, TW (Shimwell, Timothy W.); Rottgering, HJA (Rottgering, Huub J. A.); Bonafede, A (Bonafede, Annalisa); Botteon, A (Botteon, Andrea); Cuciti, V (Cuciti, Virginia); Dallacasa, D (Dallacasa, Daniele); de Gasperin, F (de Gasperin, Francesco); Dominguez-Fernandez, P (Dominguez-Fernandez, Paola); Ensslin, TA (Ensslin, Torsten A.); Gastaldello, F (Gastaldello, Fabio); Mandal, S (Mandal, Soumyajit); Rossetti, M (Rossetti, Mariachiara); Simionescu, A (Simionescu, Aurora)

**Source:** NATURE ASTRONOMY **DOI:** 10.1038/s41550-020-01244-5 **Early Access Date:** NOV 2020

**Abstract:** In the present-day Universe, magnetic fields pervade galaxy clusters(1) and have strengths of a few microgauss, as measured from Faraday rotation(2). Evidence for cluster magnetic fields is also provided by the observation of megaparsec-scale radio emission, namely radio halos and relics(3). These are commonly found in merging systems(4) and are characterized by a steep radio spectrum  $S_{\nu} \propto \nu^{-\alpha}$ , where  $S_{\nu}$  is proportional to  $\nu^{\alpha}$  and  $\nu$  is the observing frequency. It is widely believed that magneto-hydrodynamical turbulence and shock waves (re-)accelerate cosmic rays(5) and produce radio halos and relics. The origin and amplification of magnetic fields in clusters is not well understood. It has been proposed that turbulence drives a small-scale dynamo(6-11) that amplifies seed magnetic fields (which are primordial and/or injected by galactic outflows, such as active galactic nuclei, starbursts or winds(12)). At high redshift, radio halos are expected to be faint, owing to losses from inverse Compton scattering and the dimming effect with distance. Moreover, Faraday rotation measurements are difficult to obtain. If detected, distant radio halos provide an alternative tool to investigate magnetic field amplification. Here, we report Low Frequency Radio Array observations that reveal diffuse radio emission in massive clusters when the Universe was only half of its present age, with a sample occurrence fraction of about 50%. The high radio luminosities indicate that these clusters have similar magnetic field strengths to those in nearby clusters, and suggest that magnetic field amplification is fast during the first phases of cluster formation.

LOFAR reveals diffuse radio emission in massive high-redshift clusters, whose high radio luminosities indicate magnetic field strengths similar to those in nearby clusters, suggesting fast magnetic field amplification in the early Universe.

**Accession Number:** WOS:000584332300002

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Ensslin, Torsten		0000-0001-5246-1624
Bonafede, Annalisa		0000-0002-5068-4581
van Weeren, Reinout		0000-0002-0587-1660

**ISSN:** 2397-3366

**Record 126 of 236**

**Title:** Unexpected variations in posttranscriptional gene silencing induced by differentially produced dsRNAs in tobacco cells

**Author(s):** Cermak, V (Cermak, Vojtech); Tyc, D (Tyc, Dimitrij); Pribylova, A (Pribylova, Adela); Fischer, L (Fischer, Lukas)

Source: BIOCHIMICA ET BIOPHYSICA ACTA-GENE REGULATORY MECHANISMS Volume: 1863 Issue: 11 Article Number: 194647 DOI: 10.1016/j.bbagr.2020.194647 Published: NOV 2020

**Abstract:** In plants, posttranscriptional gene silencing (PTGS) is induced by small RNAs (sRNAs) generated from various dsRNA precursors. To assess the impact of dsRNA origin, we compared downregulation of GFP expression triggered by inverted repeat (IR), antisense (AS) and unterminated sense (UT) transcripts transiently expressed from the estradiol-inducible promoter. The use of homogeneously responding tobacco BY-2 cell lines allowed monitoring the onset of silencing and its reversibility. In this system, IR induced the strongest and fastest silencing accompanied by dense DNA methylation. At low induction, silencing in individual cells was binary (either strong or missing), suggesting that a certain threshold sRNA level had to be exceeded. The AS variant specifically showed a deviated sRNA-strand ratio shifted in favor of antisense orientation. In AS lines and weakly induced IR lines, only the silencer DNA was methylated, but the same target GFP sequence was not, showing that DNA methylation accompanying PTGS was influenced both by the level and origin of sRNAs, and possibly also by the epigenetic state of the locus. UT silencing appeared to be the least effective and resembled classical sense PTGS. The best responding UT lines behaved relatively heterogeneously possibly due to complexly arranged TDNA insertions. Unlike IR and AS variants that fully restored GFP expression upon removal of the inducer, only partial reactivation was observed in some UT lines. Our results pointed out several not yet described phenomena and differences between the long-known silencer variants that may direct further research and affect selection of proper silencer variants for specific applications.

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PubMed ID: 33127485

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Cermak, Vojtech		0000-0001-9466-3654

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Record 127 of 236

**Title:** SQM/COSMO Scoring Function: Reliable Quantum-Mechanical Tool for Sampling and Ranking in Structure-Based Drug Design

**Author(s):** Pecina, A (Pecina, Adam); Eyrilmez, SM (Eyrilmez, Saltuk M.); Kopruluoglu, C (Koepruelueoglu, Cemal); Miriyala, VM (Miriyala, Vijay Madhav); Lepsik, M (Lepsik, Martin); Fanfrik, J (Fanfrik, Jindrich); Rezac, J (Rezac, Jan); Hobza, P (Hobza, Pavel)

Source: CHEMPLUSCHEM Volume: 85 Issue: 11 Pages: 2360-2361 DOI: 10.1002/cplu.202000627 Published: NOV 2020

Accession Number: WOS:000594373800001

PubMed ID: 32986310

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pecina, Adam	K-2304-2012	0000-0003-3890-7831
Rezac, Jan	A-9107-2010	0000-0001-6849-7314
Eyrilmez, Saltuk Mustafa	L-2959-2017	0000-0003-1650-1961
Lepsik, Martin	C-6614-2012	0000-0003-2607-8132
Fanfrik, Jindrich		0000-0002-1257-1201

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Record 128 of 236

**Title:** From Synthetic to Biological Fe4S4 Complexes: Redox Properties Correlated to Function of Radical S-Adenosylmethionine Enzymes

**Author(s):** Bim, D (Bim, Daniel); Alonso-Gil, S (Alonso-Gil, Santiago); Srnc, M (Srnc, Martin)

Source: CHEMPLUSCHEM Volume: 85 Issue: 11 Pages: 2534-2541 DOI: 10.1002/cplu.202000663 Published: NOV 2020

**Abstract:** By employing the computational protocol for calculation of reduction potentials of the Fe4S4-containing species validated using a representative series of well-defined synthetic complexes, we focused on redox properties of two prototypical radical SAM enzymes to reveal how they transform SAM into the reactive 5'-deoxyadenosyl radical, and how they tune this radical for its proper biological function. We found the reduction potential of SAM is indeed elevated by 0.3-0.4 V upon coordination to Fe4S4, which was previously speculated in the literature. This makes a generation of 5'-deoxyadenosyl radical from SAM less endergonic (by ca. 7-9 kcal mol<sup>-1</sup>) and hence more feasible in both enzymes as compared to the identical process in water. Furthermore, our calculations indicate that the enzyme-bound 5'-deoxyadenosyl radical has a significantly lower reduction potential than in referential aqueous solution, which may help the enzymes to suppress potential side redox reactions and simultaneously elevate its proton-philic character, which may, in turn, promote the radical hydrogen-atom abstraction ability.

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PubMed ID: 33245201

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Alonso-Gil, Santiago	T-3798-2019	0000-0001-7596-8161

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Record 129 of 236

**Title:** Candidate Gene Markers Associated with Fecal Shedding of the Feline Enteric Coronavirus (FECV)

**Author(s):** Bubenikova, J (Bubenikova, Jana); Vrabelova, J (Vrabelova, Jana); Stejskalova, K (Stejskalova, Karla); Futas, J (Futas, Jan); Plasil, M (Plasil, Martin); Cerna, P (Cerna, Petra); Oppelt, J (Oppelt, Jan); Lobova, D (Lobova, Dana); Molinkova, D (Molinkova, Dobromila); Horin, P (Horin, Petr)

Source: PATHOGENS Volume: 9 Issue: 11 Article Number: 958 DOI: 10.3390/pathogens9110958 Published: NOV 2020

**Abstract:** The Feline coronavirus (FCoV) can cause a fatal disease, the Feline Infectious Peritonitis. Persistent shedders represent the most important source of infection. The role of the host in FCoV fecal shedding is unknown. The objective of this study was to develop gene markers and to test their associations with FCoV shedding patterns. Fecal samples were taken from 57 cats of 12 breeds on the day 0 and after 2, 4 and 12 months. Variation from persistent and/or high-intensity shedding to no shedding was observed. Thirteen immunity-related genes were selected as functional and positional/functional candidates. Positional candidates were selected in a candidate region detected by a GWAS analysis. Tens to hundreds of single nucleotide polymorphisms (SNPs) per gene were identified using next generation sequencing. Associations with different phenotypes were assessed by chi-square and Fisher's exact tests. SNPs of one functional and one positional candidate (NCR1 and SLX4IP, respectively) and haplotypes of four genes (SNX5, NCR2, SLX4IP, NCR1) were associated with FCoV shedding at  $p(\text{corrected}) < 0.01$ . Highly significant associations were observed for extreme phenotypes (persistent/high-intensity shedders and non-shedders) suggesting that there are two major phenotypes associated with different genotypes, highly susceptible cats permanently shedding high amounts of viral particles and resistant non-shedders.

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PubMed ID: 33213082

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Cerna, Petra	AAA-9120-2021	0000-0002-4300-8534
Plasil, Martin		0000-0003-4721-5685
Oppelt, Jan	H-7388-2017	0000-0002-3076-4840

eISSN: 2076-0817

Record 130 of 236

**Title:** A giant radio bridge connecting two galaxy clusters in Abell 1758

**Author(s):** Botteon, A (Botteon, A.); van Weeren, RJ (van Weeren, R. J.); Brunetti, G (Brunetti, G.); de Gasperin, F (de Gasperin, F.); Intema, HT (Intema, H. T.); Osinga, E (Osinga, E.); Di Gennaro, G (Di Gennaro, G.); Shimwell, TW (Shimwell, T. W.); Bonafede, A (Bonafede, A.); Bruggen, M (Brueggen, M.); Cassano, R (Cassano, R.); Cuciti, V (Cuciti, V); Dallacasa, D (Dallacasa, D.); Gastaldello, F (Gastaldello, F.); Mandal, S (Mandal, S.); Rossetti, M (Rossetti, M.); Rottgering, HJA (Rottgering, H. J. A.)

Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY Volume: 499 Issue: 1 Pages: L11-L15 DOI: 10.1093/mnras/slaa142 Published: NOV 2020

**Abstract:** Collisions between galaxy clusters dissipate enormous amounts of energy in the intracluster medium (ICM) through turbulence and shocks. In the process, Mpc-scale diffuse synchrotron emission in form of radio haloes and relics can form. However, little is known about the very early phase of the collision. We used deep radio observations from 53 MHz to 1.5 GHz to study the pre-merging galaxy clusters A1758N and A1758S that are similar to 2 Mpc apart. We confirm the presence of a giant bridge of radio emission connecting the two



systems that was reported only tentatively in our earlier work. This is the second large-scale radio bridge observed to date in a cluster pair. The bridge is clearly visible in the LOFAR image at 144 MHz and tentatively detected at 53 MHz. Its mean radio emissivity is more than one order of magnitude lower than that of the radio haloes in A1758N and A1758S. Interestingly, the radio and X-ray emissions of the bridge are correlated. Our results indicate that non-thermal phenomena in the ICM can be generated also in the region of compressed gas in-between infalling systems.

**Accession Number:** WOS:000587776700003

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
BOTTEON, ANDREA		0000-0002-9325-1567
Bonafede, Annalisa		0000-0002-5068-4581
van Weeren, Reinout		0000-0002-0587-1660

ISSN: 0035-8711

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#### Record 131 of 236

**Title:** Antiferromagnetic CuMnAs: Ab initio description of finite temperature magnetism and resistivity

**Author(s):** Wagenknecht, D (Wagenknecht, David); Vyborny, K (Vyborny, Karel); Carva, K (Carva, Karel); Turek, I (Turek, Ilja)

**Source:** JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 513 **Article Number:** 167078 **DOI:** 10.1016/j.jmmm.2020.167078 **Published:** NOV 1 2020

**Abstract:** Noncollinear magnetic moments in antiferromagnets (AFM) lead to a complex behavior of electrical transport, even to a decreasing resistivity due to an increasing temperature. Proper treatment of such phenomena is required for understanding AFM systems at finite temperatures; however first-principles description of these effects is complicated. With ab initio techniques, we investigate three models of spin fluctuations (magnons) influencing the transport in AFM CuMnAs; the models are numerically feasible and easily implementable to other studies. We numerically justified a fully relativistic collinear disordered local moment approach and we present its uncompensated generalization. A saturation or a decrease of resistivity caused by magnons, phonons, and their combination (above approx. 400 K) was observed and explained by changes in electronic structure. Within the coherent potential approximation, our finite-temperature approaches may be applied also to systems with impurities, which are found to have a large impact not only on residual resistivity, but also on canting of magnetic moments from the AFM to the ferromagnetic (FM) state.

**Accession Number:** WOS:000562015200008

**Author Identifiers:**

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

ISSN: 0304-8853

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#### Record 132 of 236

**Title:** Physical and dynamical characterization of the Euphrosyne asteroid family

**Author(s):** Yang, B (Yang, B.); Hanus, J (Hanus, J.); Broz, M (Broz, M.); Chrenko, O (Chrenko, O.); Willman, M (Willman, M.); Sevecek, P (Sevecek, P.); Masiero, J (Masiero, J.); Kaluna, H (Kaluna, H.)

**Source:** ASTRONOMY & ASTROPHYSICS **Volume:** 643 **Article Number:** A38 **DOI:** 10.1051/0004-6361/202038567 **Published:** OCT 29 2020

**Abstract:** Aims. The Euphrosyne asteroid family occupies a unique zone in orbital element space around 3.15 au and may be an important source of the low-albedo near-Earth objects. The parent body of this family may have been one of the planetesimals that delivered water and organic materials onto the growing terrestrial planets. We aim to characterize the compositional properties as well as the dynamical properties of the family.

**Methods:** We performed a systematic study to characterize the physical properties of the Euphrosyne family members via low-resolution spectroscopy using the NASA Infrared Telescope Facility. In addition, we performed smoothed-particle hydrodynamics (SPH) simulations and N-body simulations to investigate the collisional origin, determine a realistic velocity field, study the orbital evolution, and constrain the age of the Euphrosyne family.

**Results:** Our spectroscopy survey shows that the family members exhibit a tight taxonomic distribution, suggesting a homogeneous composition of the parent body. Our SPH simulations are consistent with the Euphrosyne family having formed via a reaccumulation process instead of a cratering event. Finally, our N-body simulations indicate that the age of the family is 280+180 80 Myr, which is younger than previous estimates.

**Accession Number:** WOS:000591362600001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Chrenko, Ondrej	G-3516-2017	0000-0001-7215-5026
Masiero, Joseph		0000-0003-2638-720X

ISSN: 0004-6361

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#### Record 133 of 236

**Title:** Liquid-Phase Exfoliated GeSe Nanoflakes for Photoelectrochemical-Type Photodetectors and Photoelectrochemical Water Splitting

**Author(s):** Bianca, G (Bianca, Gabriele); Zappia, MI (Zappia, Marilena I.); Bellani, S (Bellani, Sebastiano); Sofer, ZK (Sofer, Zdene. K.); Serri, M (Serri, Michele); Najafi, L (Najafi, Leyla); Oropesa-Nunez, R (Oropesa-Nunez, Reinier); Martin-Garcia, B (Martin-Garcia, Beatriz); Hartman, T (Hartman, Tomas); Leoncino, L (Leoncino, Luca); Sedmidubsky, D (Sedmidubsky, David); Pellegrini, V (Pellegrini, Vittorio); Chiarello, G (Chiarello, Gennaro); Bonaccorso, F (Bonaccorso, Francesco)

**Source:** ACS APPLIED MATERIALS & INTERFACES **Volume:** 12 **Issue:** 43 **Pages:** 48598-48613 **DOI:** 10.1021/acsaami.0c14201 **Published:** OCT 28 2020

**Abstract:** Photoelectrochemical (PEC) systems represent powerful tools to convert electromagnetic radiation into chemical fuels and electricity. In this context, two-dimensional (2D) materials are attracting enormous interest as potential advanced photo(electro)catalysts and, recently, 2D group-IVA metal monochalcogenides have been theoretically predicted to be water splitting photocatalysts. In this work, we use density functional theory calculations to theoretically investigate the photocatalytic activity of single-/few-layer GeSe nanoflakes for both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) in pH conditions ranging from 0 to 14. Our simulations show that GeSe nanoflakes with different thickness can be mixed in the form of nanoporous films to act as nanoscale tandem systems, in which the flakes, depending on their thickness, can operate as HER- and/or OER photocatalysts. On the basis of theoretical predictions, we report the first experimental characterization of the photo(electro)catalytic activity of single-/few-layer GeSe flakes in different aqueous media, ranging from acidic to alkaline solutions: 0.5 M H<sub>2</sub>SO<sub>4</sub> (pH 0.3), 1 M KCl (pH 6.5), and 1 M KOH (pH 14). The films of the GeSe nanoflakes are fabricated by spray coating GeSe nanoflakes dispersion in 2-propanol obtained through liquid-phase exfoliation of synthesized orthorhombic (Pnma) GeSe bulk crystals. The PEC properties of the GeSe nanoflakes are used to design PEC-type photodetectors, reaching a responsivity of up to 0.32 AW<sup>-1</sup> (external quantum efficiency of 86.3%) under 455 nm excitation wavelength in acidic electrolyte. The obtained performances are superior to those of several self-powered and low-voltage solution-processed photodetectors, approaching that of self-powered commercial UV-Vis photodetectors. The obtained results inspire the use of 2D GeSe in proof-of-concept water photoelectrolysis cells.

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**PubMed ID:** 32960559

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Martin-Garcia, Beatriz	AAH-8966-2020	0000-0001-7065-856X
Serri, Michele	K-1043-2016	0000-0002-6018-5284
Leoncino, Luca		0000-0001-8561-3460

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#### Record 134 of 236

**Title:** On-Surface Synthesis of Polyferrocenylene and its Single-Chain Conformational and Electrical Transport Properties

**Author(s):** Santhini, VM (Santhini, Vijai M.); Stetsovych, O (Stetsovych, Oleksandr); Ondracek, M (Ondracek, Martin); Moreno, JMI (Mendieta Moreno, Jesus I.); Mutombo, P (Mutombo, Pingo); de la Torre, B (de la Torre, Bruno); Svec, M (Svec, Martin); Klivar, J (Klivar, Jiri); Stara, IG (Stara, Irena G.); Vazquez, H (Vazquez, Hector); Stary, I (Stary, Ivo); Jelinek, P (Jelinek, Pavel)

Source: ADVANCED FUNCTIONAL MATERIALS Article Number: 2006391 DOI: 10.1002/adfm.202006391 Early Access Date: OCT 2020

**Abstract:** Unlike intrinsically conductive organic polymers, which are central to organic electronics/photovoltaics, metallopolymers contain multiple redox-active centers allowing extra control of their intriguing properties. Ferrocene polymers are particularly attractive in this regard, but research of the iconic poly(1,1'-ferrocenylene), a main-chain ferrocene polymer with the most densely bound redox-active iron centers, has practically stopped because it is an insoluble and rather inhomogeneous material. Herein, its synthesis on the Ag(111) surface is reported, based on the Ullmann coupling of 1,1'-diiodo-1,1'-biferrocene. Conformationally flexible single-chain nanowires up to 50 nm in length, thus overcoming the limits of conventional solution polymerization, are characterized by scanning probe microscopy techniques achieving atomic resolution. Single-chain electrical conductivity measurements are performed in the longitudinal directions revealing apparent metal-to-semiconductor transition (depending on the number of ferrocene units lifted from the surface). A simple transport model is established to rationalize this observation.

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Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Moreno, Jesus I Mendieta	K-5640-2017	0000-0001-8530-3315
Jelinek, Pavel	ABE-8589-2020	0000-0002-5645-8542
De la Torre, Bruno	R-4536-2019	
Svec, Martin	G-6645-2014	0000-0003-0369-8144
de la Torre, Bruno		0000-0002-6462-6833
Mutombo, Pingo	G-5266-2014	0000-0002-8175-7587
Stetsovych, Oleksandr		0000-0001-7788-1617
Ondracek, Martin		0000-0002-8808-1487

ISSN: 1616-301X

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#### Record 135 of 236

**Title:** Migration of gap-opening planets in 3D stellar-irradiated accretion disks

**Author(s):** Chrenko, O (Chrenko, O.); Nesvorný, D (Nesvorný, D.)

Source: ASTRONOMY & ASTROPHYSICS Volume: 642 Article Number: A219 DOI: 10.1051/0004-6361/202038988 Published: OCT 23 2020

**Abstract:** Context. The origin of giant planets at moderate separations similar or equal to 1-10 au is still not fully understood because numerical studies of Type II migration in protoplanetary disks often predict a decay of the semi-major axis that is too fast. According to recent 2D simulations, inward migration of a gap-opening planet can be slowed down or even reversed if the outer gap edge becomes heated by irradiation from the central star, and puffed up. Aims. Here, we study how stellar irradiation reduces the disk-driven torque and affects migration in more realistic 3D disks. Methods. Using 3D hydrodynamic simulations with radiation transfer, we investigated the static torque acting on a single gap-opening planet embedded in a passively heated accretion disk. Results. Our simulations confirm that a temperature inversion is established at the irradiated outer gap edge and the local increase of the scale height reduces the magnitude of the negative outer Lindblad torque. However, the temperature excess is smaller than assumed in 2D simulations and the torque reduction only becomes prominent for specific parameters. For the viscosity  $\alpha = 10^{-3}$ , the total torque is reduced for planetary masses ranging from 0.1 to 0.7 Jupiter mass, with the strongest reduction being by a factor of  $\sim 0.17$  (implying outward migration) for a Saturn-mass planet. For a Jupiter-mass planet, the torque reduction becomes stronger with increasing  $\alpha$  (the torque is halved when  $\alpha = 5 \times 10^{-3}$ ). Conclusions. We conclude that planets that open moderately wide and deep gaps are subject to the largest torque modifications and their Type II migration can be stalled due to gap edge illumination. We then argue that the torque reduction can help to stabilize the orbits of giant planets forming at greater than or similar to 1 au.

Accession Number: WOS:000586584100002

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Chrenko, Ondrej	G-3516-2017	0000-0001-7215-5026

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#### Record 136 of 236

**Title:** Supernova explosions interacting with aspherical circumstellar material: implications for light curves, spectral line profiles, and polarization

**Author(s):** Kurfurst, P (Kurfurst, P.); Pejcha, O (Pejcha, O.); Krucka, J (Krticka, J.)

Source: ASTRONOMY & ASTROPHYSICS Volume: 642 Article Number: A214 DOI: 10.1051/0004-6361/202039073 Published: OCT 22 2020

**Abstract:** Some supernova (SN) explosions show evidence for an interaction with a pre-existing nonspherically symmetric circumstellar medium (CSM) in their light curves, spectral line profiles, and polarization signatures. The origin of this aspherical CSM is unknown, but binary interactions have often been implicated. To better understand the connection with binary stars and to aid in the interpretation of observations, we performed two-dimensional axisymmetric hydrodynamic simulations where an expanding spherical SN ejecta initialized with realistic density and velocity profiles collide with various aspherical CSM distributions. We consider CSM in the form of a circumstellar disk, colliding wind shells in binary stars with different orientations and distances from the SN progenitor, and bipolar lobes representing a scaled down version of the Homunculus nebula of eta Car. We study how our simulations map onto observables, including approximate light curves, indicative spectral line profiles at late times, and estimates of a polarization signature. We find that the SN-CSM collision layer is composed of normal and oblique shocks, reflected waves, and other hydrodynamical phenomena that lead to acceleration and shear instabilities. As a result, the total shock heating power fluctuates in time, although the emerging light curve might be smooth if the shock interaction region is deeply embedded in the SN envelope. SNe with circumstellar disks or bipolar lobes exhibit late-time spectral line profiles that are symmetric with respect to the rest velocity and relatively high polarization. In contrast, SNe with colliding wind shells naturally lead to line profiles with asymmetric and time-evolving blue and red wings and low polarization. Given the high frequency of binaries among massive stars, the interaction of SN ejecta with a pre-existing colliding wind shell must occur and the observed signatures could be used to characterize the binary companion.

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#### Record 137 of 236

**Title:** Transferring Lithium Ions in the Nanochannels of Flexible Metal-Organic Frameworks Featuring Superchaotropic Metallacarborane Guests: Mechanism of Ionic Conductivity at Atomic Resolution

**Author(s):** Brus, J (Brus, Jiri); Czernek, J (Czernek, Jiri); Urbanova, M (Urbanova, Martina); Rohlicek, J (Rohlicek, Jan); Plechacek, T (Plechacek, Tomas)

Source: ACS APPLIED MATERIALS & INTERFACES Volume: 12 Issue: 42 Special Issue: SI Pages: 47447-47456 DOI: 10.1021/acsami.0c12293 Published: OCT 21 2020

**Abstract:** Metal-organic frameworks (MOFs), owing to their unique architecture, attract consistent attention in the design of high-performance Li battery materials. Here, we report a new category of ion-conducting crystalline materials for all-solid-state electrolytes based on an MIL53(Al) framework featuring a superchaotropic metallacarborane (Li+CoD-) salt and present the first quantitative data on Li+ ion sites, local dynamics, chemical exchange, and the formation of charge-transfer pathways. We used multinuclear solid-state nuclear magnetic resonance (ss-NMR) spectroscopy to examine the mechanism of ionic conductivity at atomic resolution and to elucidate order-disorder processes, framework-ion interactions, and framework breathing during the loading of Li+CoD- species and transfer of Li+ ions. In this way, the MIL53(Al)@LiCoD framework was found to adopt an open-pore conformation accompanied by a minor fraction of narrow-pore channels. The inserted Li+ ions have two states (free and bound), which both exhibit extensive motions. Both types of Li+ ions form mutually communicating chains, which are large enough to enable efficient long-range charge transfer and macroscopic conductivity. The superchaotropic anions undergo high-amplitude uniaxial rotation motions supporting the transfer of Li+ cations along them, while the fluctuations of MOF aromatic linkers support the penetration of Li+ through the channel walls. Our findings provide a detailed atomic-resolution insight into the mechanism of ionic conductivity and thus have significant implications for the design of the next generation of energy-related materials.

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Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rohlicek, Jan		0000-0001-6913-2667

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#### Record 138 of 236

**Title:** Two Spectroscopies in One: Interference of Circular Dichroism and Raman Optical Activity

**Author(s):** Wu, T (Wu, Tao); Li, GJ (Li, Guojie); Kapitan, J (Kapitan, Josef); Kessler, J (Kessler, Jiri); Xu, YJ (Xu, Yunjie); Bour, P (Bour, Petr)

**Source:** ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 59 **Issue:** 49 **Pages:** 21895-21898 **DOI:** 10.1002/anie.202011146 **Early Access Date:** OCT 2020 **Published:** DEC 1 2020

**Abstract:** Previously, we and other laboratories have reported an unusual and strong Raman optical activity (ROA) induced in solvents by chiral dyes. Various theories of the phenomenon appeared, but they were not capable of explaining fully the observed ROA band signs and intensities. In this work, an analysis based both on the light scattering theory and dedicated experiments provides a more complete understanding. For example, double-cell magnetic circular dichroism and magnetic ROA experiments with copper-porphyrin complex show that the induced chirality is observed without any contact of the solvents with the complex. The results thus indicate that a combination of electronic circular dichroism (ECD) with the polarized Raman scattering is responsible for the effect. The degree of circularity of solvent vibrational bands is a principal molecular property participating in the event. The insight and the possibility to predict the chirality transfer promise future applications in spectroscopy, chemical analysis and polarized imaging.

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**PubMed ID:** 32926516

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Wu, Tao	B-3667-2010	0000-0002-0244-3046
Li, Guojie		0000-0002-9768-4212
Kapitan, Josef	E-7136-2013	0000-0002-1916-9186
Xu, Yunjie	G-6542-2014	0000-0003-3736-3190

**ISSN:** 1433-7851

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#### Record 139 of 236

**Title:** HARDI-ZOOMit protocol improves specificity to microstructural changes in presymptomatic myelopathy

**Author(s):** Labounek, R (Labounek, Rene); Valosek, J (Valosek, Jan); Horak, T (Horak, Tomas); Svatkova, A (Svatkova, Alena); Bednarik, P (Bednarik, Petr); Vojtisek, L (Vojtisek, Lubomir); Horakova, M (Horakova, Magda); Nestrail, I (Nestrail, Igor); Lenglet, C (Lenglet, Christophe); Cohen-Adad, J (Cohen-Adad, Julien); Bednarik, J (Bednarik, Josef); Hlustik, P (Hlustik, Petr)

**Source:** SCIENTIFIC REPORTS **Volume:** 10 **Issue:** 1 **Article Number:** 17529 **DOI:** 10.1038/s41598-020-70297-3 **Published:** OCT 16 2020

**Abstract:** Diffusion magnetic resonance imaging (dMRI) proved promising in patients with non-myelopathic degenerative cervical cord compression (NMDCCC), i.e., without clinically manifested myelopathy. Aim of the study is to present a fast multi-shell HARDI-ZOOMit dMRI protocol and validate its usability to detect microstructural myelopathy in NMDCCC patients. In 7 young healthy volunteers, 13 age-comparable healthy controls, 18 patients with mild NMDCCC and 15 patients with severe NMDCCC, the protocol provided higher signal-to-noise ratio, enhanced visualization of white/gray matter structures in microstructural maps, improved dMRI metric reproducibility, preserved sensitivity (SE = 87.88%) and increased specificity (SP = 92.31%) of control-patient group differences when compared to DTI-RESOLVE protocol (SE = 87.88%, SP = 76.92%). Of the 56 tested microstructural parameters, HARDI-ZOOMit yielded significant patient-control differences in 19 parameters, whereas in DTI-RESOLVE data, differences were observed in 10 parameters, with mostly lower robustness. Novel marker the white-gray matter diffusivity gradient demonstrated the highest separation. HARDI-ZOOMit protocol detected larger number of crossing fibers (5-15% of voxels) with physiologically plausible orientations than DTI-RESOLVE protocol (0-8% of voxels). Crossings were detected in areas of dorsal horns and anterior white commissure. HARDI-ZOOMit protocol proved to be a sensitive and practical tool for clinical quantitative spinal cord imaging.

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**PubMed ID:** 33067520

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Labounek, Rene	AAB-3090-2019	0000-0003-0439-1304
Nestrail, Igor	ABG-7030-2020	0000-0002-3833-1484
Horakova, Magda	B-5772-2018	0000-0003-3317-2661
Horak, Tomas	ABE-1115-2020	0000-0003-1743-1133
Valosek, Jan	X-5305-2018	0000-0002-7398-4990
Bednarik, Petr	B-3956-2014	0000-0002-8828-7661

**ISSN:** 2045-2322

#### Record 140 of 236

**Title:** Predictions for nuclear structure functions from the impact-parameter-dependent Balitsky-Kovchegov equation

**Author(s):** Cepila, J (Cepila, J.); Contreras, JG (Contreras, J. G.); Matas, M (Matas, M.)

**Source:** PHYSICAL REVIEW C **Volume:** 102 **Issue:** 4 **Article Number:** 044318 **DOI:** 10.1103/PhysRevC.102.044318 **Published:** OCT 16 2020

**Abstract:** In this work we present dipole scattering amplitudes, including the dependence on the impact-parameter, for a variety of nuclear targets of interest for the electron-ion colliders (EICs) being currently designed. These amplitudes are obtained by numerically solving the Balitsky-Kovchegov equation with the collinearly improved kernel. Two different cases are studied: initial conditions representing the nucleus under consideration and the solutions based on an initial condition representing a proton complemented by a Glauber-Gribov prescription to obtain dipole-nucleus amplitudes. We find that the energy evolution of these two approaches differ. We use the obtained dipole scattering amplitudes to predict (i) nuclear structure functions that can be measured in deep-inelastic scattering at EICs and (ii) nuclear suppression factors that reveal the energy evolution of shadowing for the different cases we studied. We compare our predictions with the available data.

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#### Record 141 of 236

**Title:** Impact of Magnetic Field Strength on Resolution and Sensitivity of Proton Resonances in Biological Solids

**Author(s):** Xue, K (Xue, Kai); Sarkar, R (Sarkar, Riddhiman); Lalli, D (Lalli, Daniela); Koch, B (Koch, Benita); Pintacuda, G (Pintacuda, Guido); Tosner, Z (Tosner, Zdenek); Reif, B (Reif, Bernd)

**Source:** JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 124 **Issue:** 41 **Pages:** 22631-22637 **DOI:** 10.1021/acs.jpcc.0c05407 **Published:** OCT 15 2020

**Abstract:** Sensitivity and resolution together determine the quality of NMR spectra in biological solids. Higher magic angle spinning frequencies yield a more efficient suppression of the coupling network and enable atomic-level investigations of protonated protein samples. On the other hand, truncation effects induced by higher magnetic fields have an impact on the achievable sensitivity and resolution. In this work, we address the question of how the proton dipolar coupling network affects the magnetic field strength-dependent gains in sensitivity and resolution. We find that beyond the canonical B-0(3/2) dependence-an additional factor of 2 in sensitivity can be achieved for residues embedded in the core of the protein, when the static magnetic field induces a transition from the strong- to the weak-coupling limit. The experiments are carried out using a selectively methyl-protonated ((13)CH3) alpha-spectrin SH3 sample, at magnetic field strengths of 11.75 T (H-1 Larmor frequency of 500 MHz) and 23.5 T (H-1 Larmor frequency of 1 GHz).

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**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Sarkar, Riddhiman		0000-0001-9055-7897

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#### Record 142 of 236

**Title:** The LOFAR view of FR 0 radio galaxies

**Author(s):** Capetti, A (Capetti, A.); Brienza, M (Brienza, M.); Baldi, RD (Baldi, R. D.); Giovannini, G (Giovannini, G.); Morganti, R (Morganti, R.); Hardcastle, MJ (Hardcastle, M. J.); Rottgering, HJA (Rottgering, H. J. A.); Brunetti, GF (Brunetti, G. F.); Best, PN (Best, P. N.); Miley, G (Miley, G.)

**Source:** ASTRONOMY & ASTROPHYSICS **Volume:** 642 **Article Number:** A107 **DOI:** 10.1051/0004-6361/202038671 **Published:** OCT 9 2020



**Abstract:** We explore the low-frequency radio properties of the sources in the Fanaro ff-Riley class 0 catalog (FROCAT) as seen by the LowFrequency ARray (LOFAR) observations at 150 MHz. This sample includes 104 compact radio active galactic nuclei (AGN) associated with nearby ( $z < 0.05$ ) massive early-type galaxies. Sixty-six FROCAT sources are in the sky regions observed by LOFAR and all of them are detected, usually showing point-like structures with sizes of 3-6 kpc. However, 12 FR 0s present resolved emission of low surface brightness, which contributes between 5% and 40% of the total radio power at 150 MHz, usually with a jetted morphology extending between 15 and 50 kpc. No extended emission is detected around the other FR 0s, with a typical luminosity limit of 5 similar to 1022WHz 1 over an area of 100 kpc X 100 kpc. The spectral slopes of FR 0s between 150MHz and 1.4 GHz span a broad range (0.7 less than or similar to .alpha less than or similar to 0:8) with a median value of ff alpha 0:1; 20% of them have a steep spectrum (alpha greater than or similar to 0:5), which is an indication of the presence of substantial extended emission confined within the spatial resolution limit. The fraction of FR 0s showing evidence for the presence of jets, by including both spectral and morphological information, is at least similar to 40%. This study confirms that FR 0s and FR 1s can be interpreted as two extremes of a continuous population of jetted sources, with the FR 0s representing the low end in size and radio power.

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**ISSN:** 0004-6361

**eISSN:** 1432-0746

#### Record 143 of 236

**Title:** Exploring the Stability of Twisted van der Waals Heterostructures

**Author(s):** Silva, A (Silva, Andrea); Claerbout, VEP (Claerbout, Victor E. P.); Polcar, T (Polcar, Tomas); Kramer, D (Kramer, Denis); Nicolini, P (Nicolini, Paolo)

**Source:** ACS APPLIED MATERIALS & INTERFACES **Volume:** 12 **Issue:** 40 **Pages:** 45214-45221 **DOI:** 10.1021/acsami.0c13971 **Published:** OCT 7 2020

**Abstract:** Recent research showed that the rotational degree of freedom in stacking 2D materials yields great changes in the electronic properties. Here, we focus on an often overlooked question: are twisted geometries stable and what defines their rotational energy landscape? Our simulations show how epitaxy theory breaks down in these systems, and we explain the observed behavior in terms of an interplay between flexural phonons and the interlayer coupling, governed by the moire superlattice. Our argument, applied to the well-studied MoS<sub>2</sub>/graphene system, rationalizes experimental results and could serve as guidance to design twistrionic devices.

**Accession Number:** WOS:000579956100083

**PubMed ID:** 32894936

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Silva, Andrea		0000-0001-6699-8115
Nicolini, Paolo	D-9151-2012	0000-0003-1324-7566

**ISSN:** 1944-8244

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#### Record 144 of 236

**Title:** Human-like telomeres in *Zostera marina* reveal a mode of transition from the plant to the human telomeric sequences

**Author(s):** Peska, V (Peska, Vratislav); Matl, M (Matl, Martin); Mandakov, T (Mandakov, Terezie); Vitales, D (Vitales, Daniel); Fajkus, P (Fajkus, Petr); Fajkus, J (Fajkus, Jiri); Garcia, S (Garcia, Sonia)

**Source:** JOURNAL OF EXPERIMENTAL BOTANY **Volume:** 71 **Issue:** 19 **Pages:** 5786-5793 **DOI:** 10.1093/jxb/eraa293 **Published:** OCT 7 2020

**Abstract:** A previous study describing the genome of *Zostera marina*, the most widespread seagrass in the Northern hemisphere, revealed some genomic signatures of adaptation to the aquatic environment such as the loss of stomatal genes, while other functions such as an algal-like cell wall composition were acquired. Beyond these, the genome structure and organization were comparable with those of the majority of plant genomes sequenced, except for one striking feature that went unnoticed at that time: the presence of human-like instead of the expected plant-type telomeric sequences. By using different experimental approaches including fluorescence in situ hybridization (FISH), genome skimming by next-generation sequencing (NGS), and analysis of non-coding transcriptome, we have confirmed its telomeric location in the chromosomes of *Z. marina*. We have also identified its telomerase RNA (TR) subunit, confirming the presence of the human-type telomeric sequence in the template region. Remarkably, this region was found to be very variable even in clades with a highly conserved telomeric sequence across their species. Based on this observation, we propose that alternative annealing preferences in the template borders can explain the transition between the plant and human telomeric sequences. The further identification of paralogues of TR in several plant genomes led us to the hypothesis that plants may retain an increased ability to change their telomeric sequence. We discuss the implications of this occurrence in the evolution of telomeres while introducing a mechanistic model for the transition from the plant to the human telomeric sequences.

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**PubMed ID:** 32589715

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Peska, Vratislav	ABE-1871-2020	0000-0002-0526-2988
Fajkus, Jiri	D-2499-2012	0000-0002-3112-1716
Matl, Martin		0000-0002-7215-3386

**ISSN:** 0022-0957

**eISSN:** 1460-2431

#### Record 145 of 236

**Title:** Alignment in the orientation of LOFAR radio sources

**Author(s):** Osinga, E (Osinga, E.); Miley, GK (Miley, G. K.); van Weeren, RJ (van Weeren, R. J.); Shimwell, TW (Shimwell, T. W.); Duncan, KJ (Duncan, K. J.); Hardcastle, MJ (Hardcastle, M. J.); Mechev, AP (Mechev, A. P.); Rottgering, HJA (Rottgering, H. J. A.); Tasse, C (Tasse, C.); Williams, WL (Williams, W. L.)

**Source:** ASTRONOMY & ASTROPHYSICS **Volume:** 642 **Article Number:** A70 **DOI:** 10.1051/0004-6361/202037680 **Published:** OCT 6 2020

**Abstract:** Various studies have laid claim to finding an alignment of the polarization vectors or radio jets of active galactic nuclei over large distances, but these results have proven controversial and so far, there is no clear explanation for this observed alignment. To investigate this case further, we tested the hypothesis that the position angles of radio galaxies are randomly oriented in the sky by using data from the Low-Frequency Array (LOFAR) Two-metre Sky Survey (LoTSS). A sample of 7555 double-lobed radio galaxies was extracted from the list of 318 520 radio sources in the first data release of LoTSS at 150 MHz. We performed statistical tests for uniformity of the two-dimensional (2D) orientations for the complete 7555 source sample. We also tested the orientation uniformity in three dimensions (3D) for the 4212 source sub-sample with photometric or spectroscopic redshifts. Our sample shows a significant deviation from uniformity ( $p$ -value  $< 10^{-5}$ ) in the 2D analysis at angular scales of about four degrees, mainly caused by sources with the largest flux densities. No significant alignment was found in the 3D analysis. Although the 3D analysis has access to fewer sources and suffers from uncertainties in the photometric redshift, the lack of alignment in 3D points towards the cause of the observed effect being unknown systematics or biases that predominantly affect the brightest sources, although this has yet to be demonstrated irrefutably and should be the subject of subsequent studies.

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**eISSN:** 1432-0746

#### Record 146 of 236

**Title:** Gallium Species Incorporated into MOF Structure: Insight into the Formation of a 3D Polycrystalline Gallium-Imidazole Framework

**Author(s):** Kobera, L (Kobera, Libor); Havlin, J (Havlin, Jakub); Abbrent, S (Abbrrent, Sabina); Rohlicek, J (Rohlicek, Jan); Streckova, M (Streckova, Magdalena); Sopcak, T (Sopcak, Tibor); Kyselova, V (Kyselova, Veronika); Czernek, J (Czernek, Jiri); Brus, J (Brus, Jiri)

**Source:** INORGANIC CHEMISTRY **Volume:** 59 **Issue:** 19 **Pages:** 13933-13941 **DOI:** 10.1021/acs.inorgchem.0c01563 **Published:** OCT 5 2020

**Abstract:** The formation of a polycrystalline 3D gallium-imidazole framework (MOF) was closely studied in three steps using ssNMR, XRPD, and TGA. In all steps, the reaction products show relatively high temperature stability up to 500 degrees C. The final product was examined by structural analysis using NMR crystallography combined with TG and BET analyses, which enabled a detailed characterization of the polycrystalline MOF system on the atomic-resolution level. Ga-71 ssNMR spectra provided valuable structural information on the coexistence of several distinct gallium species, including a tunable liquid phase. Moreover, using an NMR crystallography approach, two structurally asymmetric units of Ga(Im(6))(6-) incorporated into the thermally stable polycrystalline 3D matrix were identified. Prepared polycrystalline MOF material with polymorphic gallium species is promising for use in catalytic processes.

**Accession Number:** WOS:000580381700016

**PubMed ID:** 32935544

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kyselova, Veronika	AAD-5087-2021	
Kyselova, Veronika		0000-0003-2686-6665
Kobera, Libor	G-5237-2014	0000-0002-8826-948X
Rohlicek, Jan		0000-0001-6913-2667
Abbrent, Sabina		0000-0003-4228-4059

ISSN: 0020-1669

eISSN: 1520-510X

**Record 147 of 236****Title:** Ab initio study of chemical disorder as an effective stabilizing mechanism of bcc-based TiAl( plus Mo)**Author(s):** Abdoshahi, N (Abdoshahi, Neda); Spoerk-Erdely, P (Spoerk-Erdely, Petra); Friak, M (Friak, Martin); Mayer, S (Mayer, Svea); Sob, M (Sob, Mojmir); Holec, D (Holec, David)**Source:** PHYSICAL REVIEW MATERIALS Volume: 4 Issue: 10 Article Number: 103604 DOI: 10.1103/PhysRevMaterials.4.103604 Published: OCT 2 2020

**Abstract:** To shed a new light on the complex microstructural evolution in the Ti-Al-Mo system, we employ ab initio calculations to study bcc-fcc structural transformations of ordered beta(o)-TiAl(+Mo) and disordered beta-TiAl(+Mo) to ordered gamma-TiAl(+Mo) and hypothetically assumed disordered gamma(dis)-TiAl(+Mo) alloys, respectively. In particular, tetragonal (Bain's path) and trigonal transformations are combined with the concept of special quasirandom structures (SQS) and examined. Our calculations of the ordered phases show that the beta(o) -> gamma tetragonal transformation of TiAl is barrierless, i.e., proceeds spontaneously, reflecting the genuine structural instability of the beta(o) phase. Upon alloying of approximate to 7.4 at.% Mo, a small barrier between beta(o) and gamma-related local energy minima is formed. Yet a higher Mo content of approximate to 9 at.% leads to an opposite-direction barrierless transformation gamma -> beta(o) i.e., fully stabilizing the beta(o) phase. Considering the disordered phases, the beta(o)-Ti0.5Al0.5-xMox and gamma(dis)-Ti0.5Al0.5-xMox, are energetically very close. Importantly, for all here-considered compositions up to 11 at.% of Mo, a small energy barrier separates beta-TiAl(+Mo) and gamma(dis)-TiAl(+Mo) energy minima. Finally, a trigonal path was studied as an alternative transformation connecting disordered beta and gamma(dis)-TiAl phases, but it turns out that it exhibits an energy barrier over 60 meV/at. which, in comparison to the Bain's path with 9 meV/at. barrier, effectively disqualifies the trigonal transformation for the TiAl system.

**Accession Number:** WOS:000576705800004**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Spoerk-Erdely, Petra		0000-0002-4978-2395
Sob, Mojmir	G-6865-2011	0000-0002-5724-890X
Holec, David		0000-0002-3516-1061

ISSN: 2475-9953

**Record 148 of 236****Title:** Quantifying colour difference in animals with variable patterning**Author(s):** Drackova, T (Drackova, Tereza); Smolinsky, R (Smolinsky, Radovan); Hladovska, Z (Hladovska, Zuzana); Dolinay, M (Dolinay, Matej); Martinkova, N (Martinkova, Natalia)**Source:** JOURNAL OF VERTEBRATE BIOLOGY Volume: 69 Issue: 4 Article Number: 20029 DOI: 10.25225/jvb.20029 Published: OCT 2020

**Abstract:** Colour pattern influences behaviour and affects survival of organisms through perception of light reflectance. Spectrophotometric methods used to study colour optimise precision and accuracy of reflectance across wavelengths, while multiband photographs are generally used to assess the complexity of colour patterns. Using standardised photographs of sand lizards (*Lacerta agilis*), we compare how colours characterised using point measurements (using the photographs, but simulating spectrophotometry) on the skin differ from colours estimated by clustering pixels in the photograph of the lizard's body. By taking photographs in the laboratory and in the field, the experimental design included two 2-way comparisons. We compare point vs. colour clustering characterisation and influence of illumination in the laboratory and in the field. We found that point measurements adequately represented the dominant colour of the lizard. Where colour patterning influenced measurement geometry, image analysis outperformed point measurement with respect to stability between technical replicates on the same animal. The greater colour variation derived from point measurements increased further under controlled laboratory illumination. Both methods revealed lateral colour asymmetry in sand lizards, i.e. that colours subtly differed between left and right flank. We conclude that studies assessing the impact of colour on animal ecology and behaviour should utilise hyperspectral imaging, followed by image analysis that encompasses the whole colour pattern.

**Accession Number:** WOS:000588646400001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Martinkova, Natalia	C-2939-2008	0000-0003-4556-4363

ISSN: 2694-7684

**Record 149 of 236****Title:** Disentangling the evolutionary history of peri-Mediterranean cyprinids using host-specific gill monogeneans**Author(s):** Benovics, M (Benovics, Michal); Vukic, J (Vukic, Jasna); Sanda, R (Sanda, Radek); Rahmouni, I (Rahmouni, Imane); Simkova, A (Simkova, Andrea)**Source:** INTERNATIONAL JOURNAL FOR PARASITOLOGY Volume: 50 Issue: 12 Pages: 969-984 DOI: 10.1016/j.ijpara.2020.05.007 Published: OCT 2020

**Abstract:** The diversification of Mediterranean fish appears to be far more complex than could be explained by a single dispersion model. Cyprinids represent one of the most species-rich groups of freshwater fishes living in this region. The current distribution of several highly divergent cyprinid taxa is most likely the result of multiple dispersion events. Cyprinid fish serve as hosts for the highly diversified and host-specific monogenean parasites of the genus *Dactylogyrus*. On the assumption that the distribution of *Dactylogyrus* spp. reflects the biogeography and evolutionary history of their hosts, we used these parasites as an additional tool to shed new light on the evolutionary history of peri-Mediterranean cyprinids of the subfamily Barbinae. The degree of congruence between host and parasite phylogenies was investigated using 29 *Dactylogyrus* spp. and 34 Barbinae hosts belonging to the genera *Aulopyge*, *Barbus* and *Luciobarbus*. We showed that the morphological adaptation of *Dactylogyrus* (i.e. of the ventral bar, representing the most variable morphological character of the attachment organ) is linked with parasite phylogeny. By applying distance-based and event-based cophylogenetic approaches, we revealed a significant global coevolutionary signal. A total of 62% of individual host-parasite links contributed significantly to the coevolutionary structure evidenced between hosts of *Barbus* spp. and Iberian *Luciobarbus* spp., and their host-specific *Dactylogyrus* spp. The host switching of parasites was revealed as the most important coevolutionary event in the *Dactylogyrus*-Barbinae system in the peri-Mediterranean region. Cophylogenetic analyses and the mapping of the morphological character of the parasite attachment organ onto the phylogeny of *Dactylogyrus* indicate that endemic southern European *Dactylogyrus* spp. parasitizing cyprinids of Barbinae have multiple origins. We suggest that continental bridges connecting southern Europe and North Africa played a crucial role in the dispersion of cyprinids, affecting the distribution of their host-specific gill parasites. (C) 2020 Australian Society for Parasitology. Published by Elsevier Ltd. All rights reserved.

**Accession Number:** WOS:000582319000004**PubMed ID:** 32619430**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Benovics, Michal	AAB-7651-2021	0000-0002-4358-9332

ISSN: 0020-7519

eISSN: 1879-0135

**Record 150 of 236****Title:** Side-channel countermeasures utilizing dynamic logic reconfiguration: Protecting AES/Rijndael and Serpent encryption in hardware**Author(s):** Socha, P (Socha, Petr); Brejnik, J (Brejnik, Jan); Balasch, J (Balasch, Josep); Novotny, M (Novotny, Martin); Mentens, N (Mentens, Nele)**Source:** MICROPROCESSORS AND MICROSYSTEMS Volume: 78 Article Number: 103208 DOI: 10.1016/j.micpro.2020.103208 Published: OCT 2020

**Abstract:** Dynamic logic reconfiguration is a concept that allows for efficient on-the-fly modifications of combinational circuit behavior in both ASIC and FPGA devices. The reconfiguration of Boolean functions is achieved by modification of their generators (e.g., shift register-based look-up tables) and it can be controlled from within the chip, without the necessity of any external intervention. This hardware polymorphism can be utilized for the implementation of side-channel attack countermeasures, as demonstrated by Sasdrich et al. for the lightweight cipher PRESENT.

In this work, we adapt these countermeasures to two of the AES finalists, namely Rijndael and Serpent. Just like PRESENT, both Rijndael and Serpent are block ciphers based on a substitution-permutation network. We describe the countermeasures and adjustments necessary to protect these ciphers using the resources available in modern Xilinx FPGAs. We describe our implementations and evaluate the side-channel leakage and effectiveness of different countermeasures combinations using a methodology based on Welch's t-test. Furthermore, we attempt to break the protected AES/Rijndael implementation using second-order DPA/CPA attacks.

We did not detect any significant first-order leakage from the fully protected versions of our implementations. Using one million power traces, we detect second-order leakage from Serpent encryption, while AES encryption second-order leakage is barely detectable. We show that the countermeasures proposed by Sasdrich et al. are, with some modifications, successfully applicable to AES and Serpent.

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Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Novotny, Martin		0000-0001-6446-7257

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## Record 151 of 236

**Title:** From the vapor-liquid equilibrium to the supercritical condition. Molecular dynamics modeling of 1,3-butadiene**Author(s):** Rozsa, ZB (Rozsa, Zsafia Borbala); Minofar, B (Minofar, Babak); Reha, D (Reha, David); Viskolcz, B (Viskolcz, Bela); Szori, M (Szori, Milan)**Source:** JOURNAL OF MOLECULAR LIQUIDS **Volume:** 315 **Article Number:** 113702 **DOI:** 10.1016/j.molliq.2020.113702 **Published:** OCT 1 2020**Abstract:** Molecular interactions encode macroscopic phenomena. Molecular dynamics simulations (MD) based on classical force fields can provide structural and energetic information about phase equilibrium at different conditions as well as about systems above the critical point. In this study, vapor/liquid interface of 1,3-butadiene is investigated using classical MD and Two Phase Molecular Dynamics (2PMD) techniques in order to test force field parameters as well as to analyze structural and energetic details from ambient conditions to the supercritical phase. A new approach is proposed based on Voronoi-tessellation to categorize vapor, liquid and 'phase transferring' molecules. The force field (OPTS-AA with 1.14<sup>°</sup>CM1A partial atomic charges) combined with the 2 phi MD method is used to reproduce experimental data (density and surface tension) of 1,3-butadiene well for all investigated phases. Density (rho), potential energy (E-pot), surface tension (gamma) and specific surface area (SSA) based methods have also been tested to calculate the critical parameters of the molecular system. It is found that the density based approach is the best alternative for retrieving experimental data for the critical point (T-c, T-exp = 425.0 K, rho(c,exp) = 245 kg/m<sup>3</sup>), P-c, P-exp = 43.2 bar and T-c, T-rho = 430.25 +/- 2.50 K, rho(c,rho) = 234.25 = 2.66 kg/m<sup>3</sup>), P-c, P-rho = 39.09 +/- 0.73 bar), while from the SSA and potential energy the critical temperature can be reproduced within 1% of deviation (T-c, T-SSA = 426.5, T-c, Epot = 426.0 K). (C) 2020 Elsevier B.V. All rights reserved.**Accession Number:** WOS:000574571700009**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Reha, David		0000-0002-9500-0569

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eISSN: 1873-3166

## Record 152 of 236

**Title:** Peculiar Magnetic and Transport Properties of CuFeS<sub>2</sub>: Defects Play a Key Role**Author(s):** Navratil, J (Navratil, Jiri); Levinsky, P (Levinsky, Petr); Hejtmanek, J (Hejtmanek, Jiri); Pashchenko, M (Pashchenko, Mariia); Knizek, K (Knizek, Karel); Kubickova, L (Kubickova, Lenka); Kmjec, T (Kmjec, Tomas); Drasar, C (Drasar, Cestmir)**Source:** JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 124 **Issue:** 38 **Pages:** 20773-20783 **DOI:** 10.1021/acs.jpcc.0c06490 **Published:** SEP 24 2020**Abstract:** Our study targets some of the long-standing questions concerning the somewhat mysterious properties of chalcopyrite CuFeS<sub>2</sub>. We show that defect chemistry in connection with charge transfer within the structure is responsible for the unusual electronic and magnetic properties of CuFeS<sub>2</sub>. Specifically, our model addresses weak ferromagnetism and the high mobility of carriers on the background of a rigid antiferromagnetic structure. We show that defect structure can, counterintuitively, boost the mobility of free carriers due to defect-modified charge transfer. Further, the defect-modified charge transfer induces the weak ferromagnetism both in the Cu- and Fe-sublattice. This new view opens up space for further investigations and applications of charge transfer compounds.**Accession Number:** WOS:000575823600015**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pashchenko, Mariia I	K-4258-2017	0000-0003-2789-051X
Navratil, Jiri	N-3289-2019	0000-0002-8697-9912
Kmjec, Tomas	C-2653-2017	0000-0002-9739-1612
Hejtmanek, Jiri	G-5591-2014	0000-0001-8248-3912

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## Record 153 of 236

**Title:** Chelating Polymers for Hereditary Hemochromatosis Treatment**Author(s):** Groborz, O (Groborz, Ondrej); Polakova, L (Polakova, Lenka); Kolouchova, K (Kolouchova, Kristyna); Svec, P (Svec, Pavel); Loukotova, L (Loukotova, Lenka); Miriyala, VM (Miriya, Vijay Madhav); Francova, P (Francova, Pavla); Kucka, J (Kucka, Jan); Krijt, J (Krijt, Jan); Paral, P (Paral, Petr); Bajecny, M (Bajecny, Martin); Heizer, T (Heizer, Tomas); Pohl, R (Pohl, Radek); Dunlop, D (Dunlop, David); Czernek, J (Czernek, Jiri); Sefc, L (Sefc, Ludek); Benes, J (Benes, Jiri); Stepanek, P (Stepanek, Petr); Hobza, P (Hobza, Pavel); Hruby, M (Hruby, Martin)**Source:** MACROMOLECULAR BIOSCIENCE **Volume:** 20 **Issue:** 12 **Article Number:** 2000254 **DOI:** 10.1002/mabi.202000254 **Early Access Date:** SEP 2020 **Published:** DEC 2020**Abstract:** Hemochromatosis (iron overload) encompasses a group of diseases that are characterized by a toxic hyperaccumulation of iron in parenchymal organs. Currently, only few treatments for this disease have been approved; however, all these treatments possess severe side effects. In this study, a paradigm for hemochromatosis maintenance/preventive therapy is investigated: polymers with negligible systemic biological availability form stable complexes with iron ions in the gastrointestinal tract, which reduces the biological availability of iron. Macroporous polymer beads are synthesized with three different iron-chelating moieties (benzene-1,2-diol, benzene-1,2,3-triol, and 1,10-phenanthroline). The polymers rapidly chelate iron ions from aqueous solutions in vitro in the course of minutes, and are noncytotoxic and nonprooxidant. Moreover, the in vivo biodistribution and pharmacokinetics show a negligible uptake from the gastrointestinal tract (using <sup>125</sup>I-labeled polymer and single photon emission computed tomography/computed tomography), which generally prevents them from having systemic side effects. The therapeutic efficacy of the prepared polymers is successfully tested in vivo, and exhibits a significant inhibition of iron uptake from the gastrointestinal tract without any noticeable signs of toxicity. Furthermore, an in silico method is developed for the prediction of chelator selectivity. Therefore, this paradigm can be applied to the next-generation maintenance/preventive treatment for hemochromatosis and/or other diseases of similar pathophysiology.**Accession Number:** WOS:000571110400001**PubMed ID:** 32954629**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Groborz, Ondrej	AAA-7995-2020	0000-0002-3164-6168
Heizer, Tomas	F-7138-2017	0000-0002-6294-2939
Loukotova, Lenka		0000-0002-8087-1425
Pohl, Radek		0000-0001-7898-946X

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## Record 154 of 236

**Title:** Calculated relative populations for the Eu@C-84 isomers**Author(s):** Slanina, Z (Slanina, Zdenek); Uhlik, F (Uhlik, Filip); Bao, LP (Bao, Lipiao); Akasaka, T (Akasaka, Takeshi); Lu, X (Lu, Xing); Adamowicz, L (Adamowicz, Ludwik)**Source:** FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES **Volume:** 29 **Issue:** 2 **Pages:** 144-148 **DOI:** 10.1080/1536383X.2020.1817900 **Early Access Date:** SEP 2020 **Published:** SEP 30 2020**Abstract:** Relative populations of eight low-potential-energy IPR (isolated-pentagon-rule) isomers of Eu@C-84 are computed using the Gibbs energy based on the B2PLYPD/SDD potential energy. The calculations agree with the recent observation that the major isomer is Eu@C-2(13)-C-84 and the minor isomer is Eu@C-2(11)-C-84. There are also other two minor isomers suggested by the calculations. Insufficient solubility during soot extractions could explain why the two other minor species could not be isolated.**Accession Number:** WOS:000570270800001

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## Record 155 of 236

**Title:** Maximum Achievable N Content in Atom-by-Atom Growth of Amorphous Si-C-N**Author(s):** Houska, J (Houska, Jiri)**Source:** ACS APPLIED MATERIALS & INTERFACES **Volume:** 12 **Issue:** 37 **Pages:** 41666-41673 **DOI:** 10.1021/acsami.0c08300 **Published:** SEP 16 2020

**Abstract:** The maximum achievable N content in atom-by-atom growth of Si-C-N films is examined by combining ab initio molecular dynamics simulations in a wide range of compositions and densities with experimental data. When and only when the simulation algorithm allows the formation and final presence of N-2 molecules, the densities leading to the deepest local energy minima are in agreement with the experiment. The main attention is paid to unbonded N-2 molecules, with the aim to predict and explain the maximum content of N bonded in the amorphous networks. There are significant differences resulting from different compositions, ranging from no N-2 at the lowest energy density of a-Si3N4 (57 atom % of bonded N) to many N-2 at the lowest energy density of a-C3N4 (42 atom % of bonded N). The theoretical prediction is in agreement with the experimental results of reactive magnetron sputtering at varied Si+C sputter target compositions and N-2 partial pressures. A detailed analysis reveals that while there is a relationship between the N-2 formation and the packing factor, which is valid in the whole compositional range investigated, the lowest-energy packing factor depends on the composition. The results are important for the explanation of experimentally reported maximum N contents, design of technologically important amorphous nitrides and pathways of their preparation, prediction of their stability, and identification of what may or may not be achieved in this field.

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**PubMed ID:** 32830493

**Author Identifiers:**

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

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#### Record 156 of 236

**Title:** From pi Bonds without sigma Bonds to the Longest Metal-Metal Bond Ever: A Survey on Actinide-Actinide Bonding in Fullerenes

**Author(s):** Jaros, A (Jaros, Adam); Foroutan-Nejad, C (Foroutan-Nejad, Cina); Straka, M (Straka, Michal)

**Source:** INORGANIC CHEMISTRY Volume: 59 Issue: 17 Pages: 12608-12615 DOI: 10.1021/acs.inorgchem.0c01713 Published: SEP 8 2020

**Abstract:** Actinide actinide bonds are rare. Only a few experimental systems with An-An bonds have been described so far. Recent experimental characterization of the u(2)@l-h(7) C-80 (I. Am. Chem. Soc. 2018, 140, 3907) system with one -electron two-center (OETC) U-U bonds as was predicted by some of us (Phys. Chem. Chem. Phys. 2015, 17, 24182) encourages the search for more examples of actinide actinide bonding in fullerene cages. Here, we investigate actinide actinide bonding in An(2)@D(5h)2(1)-C-70, An(2)@l-h(7)-C-80, and An(2)@D-5h(1)-C-90 (An = Ac Cm) endohedral metallofullerenes (EMFs). Using different methods of the chemical bonding analysis, we show that most of the studied An2@C70 and An2@C80 systems feature one or more one -electron two-center actinide actinide bonds. Unique bonding patterns are revealed in plutonium EMFs. The Pu-2@l-h(7)-C-80 features two OETC Pu-Pu pi bonds without any evidence of a corresponding a bond. In the Pu-2@D-5h(1)-C-90 with r(Pu-Pu) = 5.9 angstrom, theory predicts the longest metal metal bond ever described. Predicted systems are thermodynamically stable and should be, in principle, experimentally accessible, though radioactivity of studied metals may be a serious obstacle.

**Accession Number:** WOS:000570979900079

**PubMed ID:** 32845126

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Straka, Michal	E-5246-2011	0000-0002-7857-4990
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173
Jaros, Adam	S-1987-2017	0000-0001-8605-0209

ISSN: 0020-1669

eISSN: 1520-510X

#### Record 157 of 236

**Title:** Environmental determinants of the distribution of planktonic diplomonads and kinetoplastids in the oceans

**Author(s):** Flegontova, O (Flegontova, Olga); Flegontov, P (Flegontov, Pavel); Londono, PAC (Londono, Paula Andrea Castaneda); Walczowski, W (Walczowski, Waldemar); Santic, D (Santic, Danijela); Edgcomb, VP (Edgcomb, Virginia P.); Lukes, J (Lukes, Julius); Horak, A (Horak, Ales)

**Source:** ENVIRONMENTAL MICROBIOLOGY Volume: 22 Issue: 9 Pages: 4014-4031 DOI: 10.1111/1462-2920.15190 Early Access Date: SEP 2020 Published: SEP 2020

**Abstract:** We analysed a widely used barcode, the V9 region of the 18S rRNA gene, to study the effect of environmental conditions on the distribution of two related heterotrophic protistan lineages in marine plankton, kinetoplastids and diplomonads. We relied on a major published dataset (Tara Oceans) where samples from the mesopelagic zone were available from just 32 of 123 locations, and both groups are most abundant in this zone. To close sampling gaps and obtain more information from the deeper ocean, we collected 57 new samples targeting especially the mesopelagic zone. We sampled in three geographic regions: the Arctic, two depth transects in the Adriatic Sea, and the anoxic Cariaco Basin. In agreement with previous studies, both protist groups are most abundant and diverse in the mesopelagic zone. In addition to that, we found that their abundance, richness, and community structure also depend on geography, oxygen concentration, salinity, temperature, and other environmental variables reflecting the abundance of algae and nutrients. Both groups studied here demonstrated similar patterns, although some differences were also observed. Kinetoplastids and diplomonads prefer tropical regions and nutrient-rich conditions and avoid high oxygen concentration, high salinity, and high density of algae.

**Accession Number:** WOS:000566773600001

**PubMed ID:** 32779301

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lukes, Julius	H-6760-2012	0000-0002-0578-6618
Walczowski, Waldemar		0000-0002-0243-3307

ISSN: 1462-2912

eISSN: 1462-2920

#### Record 158 of 236

**Title:** A Molecular-Level Picture of Electrospinning

**Author(s):** Jirsak, J (Jirsak, Jan); Pokorny, P (Pokorny, Pavel); Holec, P (Holec, Pavel); Dedicova, S (Dedicova, Sarka)

**Source:** WATER Volume: 12 Issue: 9 Article Number: 2577 DOI: 10.3390/w12092577 Published: SEP 2020

**Abstract:** Electrospinning is a modern and versatile method of producing nanofibers from polymer solutions or melts by the action of strong electric fields. The complex, multiscale nature of the process hinders its theoretical understanding, especially at the molecular level. The present article aims to contribute to the fundamental picture of the process by the molecular modeling of its nanoscale analogue and complements the picture by laboratory experiments at macroscale. Special attention is given to how the process is influenced by ions. Molecular dynamics (MD) is employed to model the time evolution of a nanodroplet of aqueous poly(ethylene glycol) (PEG) solution on a solid surface in a strong electric field. Two molecular weights of PEG are used, each in 12 aqueous solutions differing by the weight fraction of the polymer and the concentration of added NaCl. Various structural and dynamic quantities are monitored in production trajectories to characterize important features of the process and the effect of ions on it. Complementary experiments are carried out with macroscopic droplets of compositions similar to those used in MD. The behavior of droplets in a strong electric field is monitored using an oscilloscopic method and high-speed camera recording. Oscilloscopic records of voltage and current are used to determine the characteristic onset times of the instability of the meniscus as the times of the first discharge. The results of simulations indicate that, at the molecular level, the process is primarily driven by polarization forces and the role of ionic charge is only minor. Ions enhance the evaporation of solvent and the transport of polymer into the jet. Experimentally measured instability onset times weakly decrease with increasing ionic concentration in solutions with low polymer content. High-speed photography coupled with oscilloscopic measurement shows that the measured instability onset corresponds to the formation of a sharp tip of the Taylor cone. Molecular-scale and macroscopic views of the process are confronted, and challenges for their reconciliation are presented as a route to a true understanding of electrospinning.

**Accession Number:** WOS:000580120300001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Jirsak, Jan	A-7434-2013	0000-0003-4833-503X
Pokorny, Pavel		0000-0001-7965-3482

eISSN: 2073-4441

#### Record 159 of 236

**Title:** Searching Multiple Approximate Solutions in Configuration Space to Guide Sampling-Based Motion Planning

**Author(s):** Vonasek, V (Vonasek, Vojtech); Penicka, R (Penicka, Robert); Kozlikova, B (Kozlikova, Barbora)

**Source:** JOURNAL OF INTELLIGENT & ROBOTIC SYSTEMS **Volume:** 100 **Issue:** 3-4 **Pages:** 1527-1543 **DOI:** 10.1007/s10846-020-01247-4 **Early Access Date:** AUG 2020 **Published:** DEC 2020

**Abstract:** High-dimensional configuration space is usually searched using sampling-based motion planning methods. The well-known issue of sampling-based planners is the narrow passage problem caused by small regions of the configuration space that are difficult to cover by random samples. Practically, the presence of narrow passages decreases the probability of finding a solution, and to cope with it, the number of random samples has to be significantly increased, which also increases the planning time. By dilating the free space, e.g., by scaling-down or thinning the robot (or obstacles), narrow passages become wider, which allows us to compute an approximate solution. Then, the configuration space can be sampled densely around the approximate solution to find the solution of the original problem. However, this process may fail if the final solution is too far from the approximate one. In this paper, we propose a method to find multiple approximate solutions in the configuration space to increase the chance of finding the final solution. The approximate solutions are computed by repeated search of the configuration space while avoiding, if possible, the already discovered solutions. This enables us to search for distinct solutions leading through different parts of the configuration space. The number of approximate solutions is automatically determined based on their similarity. All approximate solutions are then used to guide the sampling of the configuration space. The performance of the proposed approach is verified in scenarios with multiple narrow passages and the benefits of the method are demonstrated by comparing the results with the state-of-the-art planners.

**Accession Number:** WOS:000564529000001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Penicka, Robert	AAI-8113-2020	0000-0001-8549-4932

ISSN: 0921-0296

eISSN: 1573-0409

#### Record 160 of 236

**Title:** Improving CT Image Tumor Segmentation Through Deep Supervision and Attentional Gates

**Author(s):** Tureckova, A (Tureckova, Alzbeta); Turecek, T (Turecek, Tomas); Oplatkova, ZK (Kominkova Oplatkova, Zuzana); Rodriguez-Sanchez, A (Rodriguez-Sanchez, Antonio)

**Source:** FRONTIERS IN ROBOTICS AND AI **Volume:** 7 **Article Number:** 106 **DOI:** 10.3389/frobt.2020.00106 **Published:** AUG 28 2020

**Abstract:** Computer Tomography (CT) is an imaging procedure that combines many X-ray measurements taken from different angles. The segmentation of areas in the CT images provides a valuable aid to physicians and radiologists in order to better provide a patient diagnosis. The CT scans of a body torso usually include different neighboring internal body organs. Deep learning has become the state-of-the-art in medical image segmentation. For such techniques, in order to perform a successful segmentation, it is of great importance that the network learns to focus on the organ of interest and surrounding structures and also that the network can detect target regions of different sizes. In this paper, we propose the extension of a popular deep learning methodology, Convolutional Neural Networks (CNN), by including deep supervision and attention gates. Our experimental evaluation shows that the inclusion of attention and deep supervision results in consistent improvement of the tumor prediction accuracy across the different datasets and training sizes while adding minimal computational overhead.

**Accession Number:** WOS:000570414900001

**PubMed ID:** 33501273

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kominkova Oplatkova, Zuzana	H-6354-2012	0000-0001-8050-162X

ISSN: 2296-9144

#### Record 161 of 236

**Title:** A Photochemical/Thermal Switch Based on 4,4'-Bis(benzimidazolium)stilbene: Synthesis and Supramolecular Properties.

**Author(s):** Kulkarni, SG (Kulkarni, Shantanu Ganesh); Jelinkova, K (Jelinkova, Kristyna); Necas, M (Necas, Marek); Pruckova, Z (Pruckova, Zdenka); Rouchal, M (Rouchal, Michal); Dastychova, L (Dastychova, Lenka); Kulhanek, P (Kulhanek, Petr); Vicha, R (Vicha, Robert)

**Source:** CHEMPHYSICHEM **Volume:** 21 **Issue:** 18 **Pages:** 2084-2095 **DOI:** 10.1002/cphc.202000472 **Early Access Date:** AUG 2020 **Published:** SEP 15 2020

**Abstract:** Stilbene derivatives are well-recognised substructures of molecular switches based on photochemically and/or thermally induced (E)/(Z) isomerisation. We combined a stilbene motif with two benzimidazolium arms to prepare new sorts of supramolecular building blocks and examined their binding properties towards cucurbit[n]urils (n=7, 8) and cyclodextrins (beta-CD, gamma-CD) in water. Based on the <sup>1</sup>H NMR data and molecular dynamics simulations, we found that two distinct complexes with different stoichiometry, i. e., guest@beta-CD and guest@beta-CD<sub>2</sub>, coexist in equilibrium in a water solution of the (Z)-stilbene-based guests. We also demonstrated that the bis(benzimidazolium)stilbene guests can be transformed from the (E) into the (Z) form via UV irradiation and back via thermal treatment in DMSO.

**Accession Number:** WOS:000563816800001

**PubMed ID:** 32672383

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Necas, Marek	F-6833-2010	
Kulhanek, Petr	D-6884-2012	0000-0002-4152-6514
Kulkarni, Shantanu		0000-0002-3919-5824
Rouchal, Michal	H-6380-2012	0000-0002-0117-4040
Pruckova, Zdenka		0000-0002-8327-6429

ISSN: 1439-4235

eISSN: 1439-7641

#### Record 162 of 236

**Title:** How Site-Directed Mutagenesis Boosted Selectivity of a Promiscuous Enzyme

**Author(s):** Nekvasilova, P (Nekvasilova, Pavlina); Kulik, N (Kulik, Natalia); Rychla, N (Rychla, Nikola); Pelantova, H (Pelantova, Helena); Petraskova, L (Petraskova, Lucie); Bosakova, Z (Bosakova, Zuzana); Cvacka, J (Cvacka, Josef); Slamova, K (Slamova, Kristyna); Kren, V (Kren, Vladimir); Bojarova, P (Bojarova, Pavla)

**Source:** ADVANCED SYNTHESIS & CATALYSIS **Volume:** 362 **Issue:** 19 **Pages:** 4138-4150 **DOI:** 10.1002/adsc.202000604 **Early Access Date:** AUG 2020 **Published:** OCT 6 2020

**Abstract:** beta-N-Acetylhexosaminidases (GH20; EC 3.2.1.52) are oxo-glycosidases with a dual activity for cleaving both N-acetylglucosamine (GlcNAc) and N-acetylgalactosamine (GalNAc) units from glycostructures. This substrate promiscuity is a hurdle in the selective synthesis of N-acetylhexosamine oligosaccharides combining both GlcNAc and GalNAc units since there are hardly any GalNAc transferring enzymes available for synthetic applications. We present here site-directed mutagenesis of a synthetically potent promiscuous beta-N-acetylhexosaminidase from *Talaromyces flavus* (TfHex), which, as a wild type, exhibits a GalNAcase/GlcNAcase ratio of 1.2. On the basis of molecular modeling, we identified crucial amino acid residues responsible for its GalNAcase/GlcNAcase selectivity. Six site-directed mutants were prepared, heterologously expressed in *Pichia pastoris*, purified, and kinetically characterized. As a result, novel engineered enzymes with an up to 7-times higher selectivity for either GalNAc or GlcNAc substrates were obtained, preserving the favorable properties of the wild type TfHex, mainly its transglycosylation potential and tolerance to functional groups in the substrate molecule. The substrate selectivity and transglycosylation yield were further corroborated by reaction engineering. The new selective and synthetically capable enzymes were applied in the preparation of tailored N-acetylhexosamines.

**Accession Number:** WOS:000563150000001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Petraskova, Lucie	F-2235-2016	0000-0002-7052-5115
Cvacka, Josef	ABC-4738-2020	0000-0002-3590-9009

ISSN: 1615-4150

eISSN: 1615-4169

#### Record 163 of 236

**Title:** Methane and carbon dioxide in dual-porosity organic matter: molecular simulations of adsorption and diffusion

**Author(s):** Rezlerova, E (Rezlerova, Eliska); Brennan, JK (Brennan, John K.); Lisl, M (Lisl, Martin)



Source: AICHE JOURNAL Article Number: e16655 DOI: 10.1002/aic.16655 Early Access Date: AUG 2020

**Abstract:** Shale gas, which predominantly consists of methane, is an important unconventional energy resource that has had a potential game-changing effect on natural gas supplies worldwide in recent years. Shale is comprised of two distinct components: organic material and clay minerals, the former providing storage for hydrocarbons and the latter minimizing hydrocarbon transport. The injection of carbon dioxide in the exchange of methane within shale formations improves the shale gas recovery, and simultaneously sequesters carbon dioxide to reduce greenhouse gas emissions. Understanding the properties of fluids such as methane and methane/carbon dioxide mixtures in narrow pores found within shale formations is critical for identifying ways to deploy shale gas technology with reduced environmental impact. In this work, we apply molecular-level simulations to explore adsorption and diffusion behavior of methane, as a proxy of shale gas, and methane/carbon dioxide mixtures in realistic models of organic materials. We first use molecular dynamics simulations to generate the porous structures of mature and overmature type-II organic matter with both micro- and mesoporosity, and systematically characterize the resulting dual-porosity organic-matter structures. We then employ the grand canonical Monte Carlo technique to study the adsorption of methane and the competing adsorption of methane/carbon dioxide mixtures in the organic-matter porous structures. We complement the adsorption studies by simulating the diffusion of adsorbed methane, and adsorbed methane/carbon dioxide mixtures in the organic-matter structures using molecular dynamics.

Accession Number: WOS:000559466400001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Lisal, Martin	A-8176-2011	0000-0001-8005-7143

ISSN: 0001-1541

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Record 164 of 236

**Title:** Multivalent Bifunctional Carbosilane Dendrimer-Supported Ammonium and Phosphonium Organocatalysts for the Coupling of CO<sub>2</sub> and Epoxides

**Author(s):** St'astna, LC (St'astna, Lucie Cervenkova); Krupkova, A (Krupkova, Alena); Petrickovic, R (Petrickovic, Roman); Mullerova, M (Mullerova, Monika); Matousek, J (Matousek, Jindrich); Kostejn, M (Kostejn, Martin); Curinova, P (Curinova, Petra); Jandova, V (Jandova, Vera); Sabata, S (Sabata, Stanislav); Strasak, T (Strasak, Tomas)

Source: ACS SUSTAINABLE CHEMISTRY & ENGINEERING Volume: 8 Issue: 31 Pages: 11692-11703 DOI: 10.1021/acssuschemeng.0c03367 Published: AUG 10 2020

**Abstract:** Insertion of carbon dioxide into the structure of organic epoxides leads to the formation of valuable cyclic carbonates and polycarbonates. For the purpose of this process, we report here a series of recyclable organocatalysts with superior activity. Carbosilane dendrimers (first to third generation) are employed as a support to which periphery ammonium or phosphonium centers are covalently attached to form a dendritic ionic liquid (DIL). The obtained DILs were tested as homogeneous catalysts in the cycloaddition of CO<sub>2</sub> to epoxides with respect to their activity and recyclability. The catalytic performance of active sites is enhanced by the presence of a proximal hydroxyl group, playing the role of a hydrogen bond donor. An experimentally observed synergistic effect was confirmed by density functional theory calculations. The activity of DILs is affected more by the structure of onium salt than by the size of the support (dendrimer generation). The dendritic catalysts of all tested generations could be recovered by nanofiltration and repeatedly reused. In order to simplify the separation of the catalysts, composite materials were prepared by intercalating the more active ammonium dendrimers into the interlayer space of a natural montmorillonite. The resulting heterogeneous catalysts were easily separable by centrifugation while retaining a reasonable level of activity.

Accession Number: WOS:000562123100022

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Stastna, Lucie Cervenkova	H-3476-2014	0000-0002-9968-1082

ISSN: 2168-0485

Record 165 of 236

**Title:** Karyotype changes in long-term cultured tick cell lines

**Author(s):** Kotsarenko, K (Kotsarenko, Kateryna); Vechtova, P (Vechtova, Pavlina); Lieskovska, J (Lieskovska, Jaroslava); Fussy, Z (Fussy, Zoltan); Cabral-de-Mello, DC (Cabral-de-Mello, Diogo C.); Rego, ROM (Rego, Ryan O. M.); Alberdi, P (Alberdi, Pilar); Collins, M (Collins, Marisol); Bell-Sakyi, L (Bell-Sakyi, Lesley); Sterba, J (Sterba, Jan); Grubhoffer, L (Grubhoffer, Libor)

Source: SCIENTIFIC REPORTS Volume: 10 Issue: 1 Article Number: 13443 DOI: 10.1038/s41598-020-70330-5 Published: AUG 10 2020

**Abstract:** Tick cell lines are an easy-to-handle system for the study of viral and bacterial infections and other aspects of tick cellular processes. Tick cell cultures are often continuously cultivated, as freezing can affect their viability. However, the long-term cultivation of tick cells can influence their genome stability. In the present study, we investigated karyotype and genome size of tick cell lines. Though 16S rDNA sequencing showed the similarity between Ixodes spp. cell lines at different passages, their karyotypes differed from 2n=28 chromosomes for parental Ixodes spp. ticks, and both increase and decrease in chromosome numbers were observed. For example, the highly passaged Ixodes scapularis cell line ISE18 and Ixodes ricinus cell lines IRE/CTVM19 and IRE/CTVM20 had modal chromosome numbers 48, 23 and 48, respectively. Also, the Ornithodoros moubata cell line OME/CTVM22 had the modal chromosome number 33 instead of 2n=20 chromosomes for Ornithodoros spp. ticks. All studied tick cell lines had a larger genome size in comparison to the genomes of the parental ticks. Thus, highly passaged tick cell lines can be used for research purposes, but possible differences in encoded genetic information and downstream cellular processes, between different cell populations, should be taken into account.

Accession Number: WOS:000561123700019

PubMed ID: 32778731

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rego, Ryan	AAL-1316-2020	0000-0001-6932-0940

ISSN: 2045-2322

Record 166 of 236

**Title:** Exploiting historical data: Pruning autotuning spaces and estimating the number of tuning steps

**Author(s):** Olha, J (Olha, Jaroslav); Hozzova, J (Hozzova, Jana); Fousek, J (Fousek, Jan); Filipovic, J (Filipovic, Jiri)

Source: CONCURRENCY AND COMPUTATION-PRACTICE & EXPERIENCE Volume: 32 Issue: 21 Special Issue: SI Article Number: e5962 DOI: 10.1002/cpe.5962 Early Access Date: AUG 2020 Published: NOV 10 2020

**Abstract:** Autotuning, the practice of automatic tuning of applications to provide performance portability, has received increased attention in the research community, especially in high performance computing. Ensuring high performance on a variety of hardware usually means modifications to the code, often via different values of a selected set of parameters, such as tiling size, loop unrolling factor, or data layout. However, the search space of all possible combinations of these parameters can be large, which can result in cases where the benefits of autotuning are outweighed by its cost, especially with dynamic tuning. Therefore, estimating the tuning time in advance or shortening the tuning time is very important in dynamic tuning applications. We have found that certain properties of tuning spaces do not vary much when hardware is changed. In this article, we demonstrate that it is possible to use historical data to reliably predict the number of tuning steps that is necessary to find a well-performing configuration and to reduce the size of the tuning space. We evaluate our hypotheses on a number of HPC benchmarks written in CUDA and OpenCL, using several different generations of GPUs and CPUs.

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Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Filipovic, Jiri	H-4311-2013	0000-0002-5703-9673

ISSN: 1532-0626

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Record 167 of 236

**Title:** New psychoactive substances on dark web markets: From deal solicitation to forensic analysis of purchased substances

**Author(s):** Jurasek, B (Jurasek, Bronislav); Cmelo, I (Cmelo, Ivan); Svoboda, J (Svoboda, Jan); Cejka, J (Cejka, Jan); Svozil, D (Svozil, Daniel); Kuchar, M (Kuchar, Martin)

Source: DRUG TESTING AND ANALYSIS Volume: 13 Issue: 1 Pages: 156-168 DOI: 10.1002/dta.2901 Early Access Date: AUG 2020 Published: JAN 2021

**Abstract:** The dark web scene has been drawing the attention of law enforcement agencies and researchers alike. To date, most of the published works on the dark web are based on data gained by passive observation. To gain a more contextualized perspective, a study was conducted in which three vendors were selected on the "Dream Market" dark web marketplace, from whom subsequently several new psychoactive substances (NPS) were ordered. All transactions were documented from the initial drug deal solicitation to the final qualitative analysis of all received samples. From the selected vendors, a total of nine NPS samples was obtained, all of which were analyzed by NMR, HRMS, LC-UV, and two also by x-ray diffraction. According to our analyses, four of the five substances offered under already known NPS names contained a different NPS. The selected vendors therefore either did

not know about their product, or deliberately deceived the buyers. Furthermore, two of three obtained samples of purportedly novel NPS were identified as already documented substances sold under a different name. However, the third characterized substance sold as "MPF-47700" was a novel, yet uncharacterized, NPS. Finally, we received a single undeclared substance, later identified as 5F-ADB. In addition to chemical analysis of the nine obtained NPS samples, the methodology used also yielded contextual information about the accessibility of NPS on the dark web, the associated purchase process, and the modus operandi of three NPS vendors. Direct participation in dark web marketplaces seems to provide additional layers of information useful for forensic studies.

**Accession Number:** WOS:000556239600001

**PubMed ID:** 32678972

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Jurasek, Bronislav	G-6493-2018	0000-0002-0262-0065
Cmelo, Ivan	AAA-9131-2021	0000-0001-7787-8653
Svoboda, Jan		0000-0003-4297-448X
Kuchar, Martin		0000-0002-7616-6352
Svozil, Daniel		0000-0003-2577-5163

**ISSN:** 1942-7603

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#### Record 168 of 236

**Title:** Ho<sub>2</sub>O@D-3(85)-C-92: Highly Stretched Cluster Dictated by a Giant Cage and Unexplored Isomerization

**Author(s):** Yu, YL (Yu, Yanling); Slanina, Z (Slanina, Zdenek); Wang, F (Wang, Feng); Yang, Y (Yang, Ying); Lian, YF (Lian, Yongfu); Uhlak, F (Uhlak, Filip); Xin, BF (Xin, Baifu); Feng, L (Feng, Lai)

**Source:** INORGANIC CHEMISTRY **Volume:** 59 **Issue:** 15 **Pages:** 11020-11027 **DOI:** 10.1021/acs.inorgchem.0c01512 **Published:** AUG 3 2020

**Abstract:** For endohedral metallofullerenes (EMFs), it has been well established that the cage shape and size should match those of the endohedral cluster. As a result, sufficient cluster-cage interaction can be achieved, which is essential for mutual stabilization. Nevertheless, how a small endohedral cluster nests in a giant fullerene has been less explored. Herein, we report a pair of large oxide-cluster fullerene (OCF) isomers, denoted as Ho<sub>2</sub>O@C-92-I and -II. Crystallographic studies reveal that major isomer-I possesses a D-3(85)-C-92 cage with a highly stretched Ho<sub>2</sub>O cluster inside, which contributes to achieving regular metal-cage contacts. Density functional theory (DFT) computations also reveal the predominant abundance of the D-3(85) isomer relative to the other two possible minor species including C-1(67) and C-2(64) isomers. Moreover, electrochemical (EC) studies verify that the isomers exhibit almost identical redox behaviors, indicating their similar cage structures. On the basis of the remarkable topological similarity of D-3(85) and C-1(67) isomers, isomer-II is likely to be Ho<sub>2</sub>O@C-1(67)-C-92, though it remains to be confirmed. Our studies thus provide new insights into the cage-cluster interplay and cage isomerization, both contributing to a better understanding of large EMFs.

**Accession Number:** WOS:000558727500064

**PubMed ID:** 32674571

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Feng, Lai	C-5186-2018	0000-0003-0278-5502

**ISSN:** 0020-1669

**eISSN:** 1520-510X

#### Record 169 of 236

**Title:** Effect of membrane composition on DivIVA-membrane interaction

**Author(s):** Jurasek, M (Jurasek, Miroslav); Flardh, K (Flardh, Klas); Vacha, R (Vacha, Robert)

**Source:** BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES **Volume:** 1862 **Issue:** 8 **Special Issue:** SI **Article Number:** 183144 **DOI:** 10.1016/j.bbmem.2019.183144 **Published:** AUG 1 2020

**Abstract:** DivIVA is a crucial membrane-binding protein that helps to localize other proteins to negatively curved membranes at cellular poles and division septa in Gram-positive bacteria. The N-terminal domain of DivIVA is responsible for membrane binding. However, to which lipids the domain binds or how it recognizes the membrane negative curvature remains elusive. Using computer simulations, we demonstrate that the N-terminal domain of *Streptomyces coelicolor* DivIVA adsorbs to membranes with affinity and orientation dependent on the lipid composition. The domain interacts non-specifically with lipid phosphates via its arginine-rich tip and the strongest interaction is with cardiolipin. Moreover, we observed a specific attraction between a negatively charged side patch of the domain and ethanolamine lipids, which addition caused the change of the domain orientation from perpendicular to parallel alignment to the membrane plane. Similar but less electrostatically dependent behavior was observed for the N-terminal domain of *Bacillus subtilis*. The domain propensity for lipids which prefer negatively curved membranes could be a mechanism for the cellular localization of DivIVA protein.

**Accession Number:** WOS:000537573200001

**PubMed ID:** 31821790

**ISSN:** 0005-2736

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#### Record 170 of 236

**Title:** The CH- $\pi$  Interaction in Protein-Carbohydrate Binding: Bioinformatics and In Vitro Quantification

**Author(s):** Houser, J (Houser, Josef); Kozmon, S (Kozmon, Stanislav); Mishra, D (Mishra, Deepti); Hammerova, Z (Hammerova, Zuzana); Wimmerova, M (Wimmerova, Michaela); Koca, J (Koca, Jaroslav)

**Source:** CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 26 **Issue:** 47 **Pages:** 10769-10780 **DOI:** 10.1002/chem.202000593 **Early Access Date:** JUL 2020 **Published:** AUG 21 2020

**Abstract:** The molecular recognition of carbohydrates by proteins plays a key role in many biological processes including immune response, pathogen entry into a cell, and cell-cell adhesion (e.g., in cancer metastasis). Carbohydrates interact with proteins mainly through hydrogen bonding, metal-ion-mediated interaction, and non-polar dispersion interactions. The role of dispersion-driven CH- $\pi$  interactions (stacking) in protein-carbohydrate recognition has been underestimated for a long time considering the polar interactions to be the main forces for saccharide interactions. However, over the last few years it turns out that non-polar interactions are equally important. In this study, we analyzed the CH- $\pi$  interactions employing bioinformatics (data mining, structural analysis), several experimental (isothermal titration calorimetry (ITC), X-ray crystallography), and computational techniques. The Protein Data Bank (PDB) has been used as a source of structural data. The PDB contains over 12 000 protein complexes with carbohydrates. Stacking interactions are very frequently present in such complexes (about 39 % of identified structures). The calculations and the ITC measurement results suggest that the CH- $\pi$  stacking contribution to the overall binding energy ranges from 4 up to 8 kcal mol<sup>-1</sup>. All the results show that the stacking CH- $\pi$  interactions in protein-carbohydrate complexes can be considered to be a driving force of the binding in such complexes.

**Accession Number:** WOS:000552350100001

**PubMed ID:** 32208534

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Koca, Jaroslav	E-4460-2012	0000-0002-2780-4901
Wimmerova, Michaela	A-4114-2010	0000-0002-7108-4198

**ISSN:** 0947-6539

**eISSN:** 1521-3765

#### Record 171 of 236

**Title:** Paramagnetic Cobalt(II) Complexes with Cyclam Derivatives: Toward F-19 MRI Contrast Agents

**Author(s):** Blahut, J (Blahut, Jan); Benda, L (Benda, Ladislav); Kotek, J (Kotek, Jan); Pintacuda, G (Pintacuda, Guido); Hermann, P (Hermann, Petr)

**Source:** INORGANIC CHEMISTRY **Volume:** 59 **Issue:** 14 **Pages:** 10071-10082 **DOI:** 10.1021/acs.inorgchem.0c01216 **Published:** JUL 20 2020

**Abstract:** In order to develop novel, more efficient, and/or selective contrast agents for magnetic resonance imaging (MRI), different modi operandi are explored as alternatives to water-relaxation enhancement. In this work, cobalt(II/III) complexes of bis(N-trifluoroethyl)cyclam derivatives with two acetate or two phosphonate pendant arms, H(2)te2f2a and H(4)te2f2p, were prepared and investigated. X-ray diffraction structures confirmed octahedral coordination with a very stable trans-III cyclam conformation and with fluorine atoms located about 5.3 angstrom from the metal center. The Co(II) complexes are kinetically inert, decomposing slowly even in 1 M aqueous HCl at 80 degrees C. The Co(II) complexes

exhibited well-resolved paramagnetically shifted NMR spectra. These were interpreted with the help of quantum chemistry calculations. The C-13 NMR shifts of the trans-[Co-II(te2f2p)](2-) complex were successfully assigned based on spin density delocalization within the ligand molecule. The obtained spin density also helps to describe d-metal-induced NMR relaxation properties of F-19 nuclei, including the contribution of a Fermi contact relaxation mechanism. The paramagnetic complexes show convenient relaxation properties to be used as F-19 MRI contrast agents.

**Accession Number:** WOS:000552287100061

**PubMed ID:** 32633944

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Hermann, Petr	A-1880-2008	0000-0001-6250-5125
Blahut, Jan	H-7494-2012	0000-0001-7752-8370
Kotek, Jan	B-1157-2017	0000-0003-1777-729X
Benda, Ladislav	D-8918-2011	0000-0003-4716-569X

ISSN: 0020-1669

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#### Record 172 of 236

**Title:** Zwitterionic Ru(III) Complexes: Stability of Metal-Ligand Bond and Host-Guest Binding with Cucurbit[7]uril

**Author(s):** Malali, S (Malali, Sanaz); Chyba, J (Chyba, Jan); Knor, M (Knor, Michal); Horni, M (Horni, Michal); Necas, M (Necas, Marek); Novotny, J (Novotny, Jan); Marek, R (Marek, Radek)

**Source:** INORGANIC CHEMISTRY **Volume:** 59 **Issue:** 14 **Pages:** 10185-10196 **DOI:** 10.1021/acs.inorgchem.0c01328 **Published:** JUL 20 2020

**Abstract:** A wide range of ruthenium-based coordination compounds have been reported to possess potential as metallo drugs with anticancer or antimetastatic activity. In this work, we synthesized a set of new zwitterionic Ru(III) compounds bearing ligands derived from N-alkyl (R) systems based on pyridine, 4,4'-bipyridine, or 1,4-diazabicyclo[2.2.2]octane (DABCO). The effects of the ligand(s) and their environment on the coordination stability have been investigated. Whereas the [DABCO-R](+) ligand is shown to be easily split out of a negative [RuCl4](-) core, positively charged R-pyridine and R-bipyridine ligands form somewhat more stable Ru(III) complexes and can be used as supramolecular anchors for binding with macrocycles. Therefore, supramolecular host-guest assemblies between the stable zwitterionic Ru(III) guests and the cucurbit[7]uril host were investigated and characterized in detail by using NMR spectroscopy and single-crystal X-ray diffraction. Paramagnetic H-1 NMR experiments supplemented by relativistic DFT calculations of the structure and hyperfine NMR shifts were performed to determine the host-guest binding modes in solution. In contrast to the intramolecular hyperfine shifts, dominated by the through-bond Fermi-contact mechanism, supramolecular hyperfine shifts were shown to depend on the "through-space" spin-dipole contributions with structural trends being satisfactorily reproduced by a simple point-dipole approximation.

**Accession Number:** WOS:000552287100073

**PubMed ID:** 32633504

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Necas, Marek	F-6833-2010	
Chyba, Jan	E-3294-2012	0000-0002-1273-5632
Novotny, Jan	D-7676-2012	0000-0002-1203-9549
Novotny, Jan	AAW-8723-2020	
Marek, Radek	D-6929-2012	0000-0002-3668-3523

ISSN: 0020-1669

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#### Record 173 of 236

**Title:** Dinucleoside Polyphosphates as RNA Building Blocks with Pairing Ability in Transcription Initiation

**Author(s):** Benoni, R (Benoni, Roberto); Culka, M (Culka, Martin); Hudecek, O (Hudecek, Oldrich); Gahurova, L (Gahurova, Lenka); Cahova, H (Cahova, Hana)

**Source:** ACS CHEMICAL BIOLOGY **Volume:** 15 **Issue:** 7 **Pages:** 1765-1772 **DOI:** 10.1021/acschembio.0c00178 **Published:** JUL 17 2020

**Abstract:** Dinucleoside polyphosphates (Np(n)Ns) were discovered 50 years ago in all cells. They are often called alarmones, even though the molecular target of the alarm has not yet been identified. Recently, we showed that they serve as noncanonical initiating nucleotides (NCINs) and fulfill the role of 5' RNA caps in Escherichia coli. Here, we present molecular insight into their ability to be used as NCINs by T7 RNA polymerase in the initiation phase of transcription. In general, we observed Np(n)Ns to be equally good substrates as canonical nucleotides for T7 RNA polymerase. Surprisingly, the incorporation of Ap(n)Gs boosts the production of RNA 10-fold. This behavior is due to the pairing ability of both purine moieties with the -1 and +1 positions of the antisense DNA strand. Molecular dynamic simulations revealed noncanonical pairing of adenosine with the thymine of the DNA.

**Accession Number:** WOS:000551550000006

**PubMed ID:** 32530599

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Cahova, Hana	O-4595-2014	0000-0002-4986-7858
Culka, Martin		0000-0002-3944-152X

ISSN: 1554-8929

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#### Record 174 of 236

**Title:** Regioselective 3-O-Substitution of Unprotected Thiodigalactosides: Direct Route to Galectin Inhibitors

**Author(s):** Vasicek, T (Vasicek, Tomas); Spiwok, V (Spiwok, Vojtech); Cerveny, J (Cerveny, Jakub); Petraskova, L (Petraskova, Lucie); Bumba, L (Bumba, Ladislav); Vrbata, D (Vrbata, David); Pelantova, H (Pelantova, Helena); Kren, V (Kren, Vladimir); Bojarova, P (Bojarova, Pavla)

**Source:** CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 26 **Issue:** 43 **Pages:** 9620-9631 **DOI:** 10.1002/chem.202002084 **Early Access Date:** JUL 2020 **Published:** AUG 3 2020

**Abstract:** The synthesis of tailored bioactive carbohydrates usually comprises challenging (de)protection steps, which lowers synthetic yields and increases time demands. We present here a regioselective single-step introduction of benzylic substituents at 3-hydroxy groups of beta-D-galactopyranosyl-(1->1)-thio-beta-D-galactopyranoside (TDG) employing dibutyltin oxide in good yields. These glycomimetics act as inhibitors of galectins-human lectins, which are biomedically attractive targets for therapeutic inhibition in, for example, cancerogenesis. The affinity of the prepared glycomimetics to galectin-1 and galectin-3 was studied in enzyme-linked immunosorbent (ELISA)-type assays and their potential to inhibit galectin binding on the cell surface was shown. We used our original in vivo biotinylated galectin constructs for easy detection by flow cytometry. The results of the biological experiments were compared with data from molecular modeling with both galectins. The present work reveals a facile and elegant synthetic route for the preparation of TDG-derived glycomimetics that exhibit differing selectivity and affinity to galectins depending on the choice of 3-O-substitution.

**Accession Number:** WOS:000546065700001

**PubMed ID:** 32368810

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Spiwok, Vojtech	A-7747-2008	0000-0001-8108-2033
Bumba, Ladislav	ABC-9943-2020	0000-0001-6659-5447
Petraskova, Lucie	F-2235-2016	0000-0002-7052-5115
Bojarova, Pavla		0000-0001-7069-0973

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#### Record 175 of 236

**Title:** Molecular characterization of Acomys louisae from Somaliland: a deep divergence and contrasting genetic patterns in a rift zone

**Author(s):** Frynta, D (Frynta, Daniel); Palupcikova, K (Palupcikova, Klara); Elmi, HSA (Elmi, Hassan Sh Abdurahman); Awale, AI (Awale, Ahmed Ibrahim); Frydlova, P (Frydlova, Petra)

**Source:** MAMMALIAN BIOLOGY **Volume:** 100 **Issue:** 4 **Pages:** 385-398 **DOI:** 10.1007/s42991-020-00045-7 **Early Access Date:** JUL 2020 **Published:** AUG 2020



**Abstract:** Phylogeographic patterns in the Horn of Africa have recently attracted researchers searching for hidden diversity and explaining the evolutionary history of this region. In this paper, we focus on spiny mouse *Acomys louisiae*. We examined 88 samples from 13 localities across Somaliland and sequenced CYTB, control region and IRBP genes. Phylogenetic analysis confirmed clear distinctness of *A. louisiae* from the other clades of *Acomys*, but it also revealed deep splits within *A. louisiae* clade. Samples from Central and Eastern Somaliland, including those from the type locality, form a clearly distinct Somaliland clade while remaining ones from the very NW of Somaliland and 5 previously published sequences from Djibouti and E Ethiopia form a Djibouti group. At two localities in the contact zone, we detected sympatric occurrence of both. The clades exhibit sharply contrasting patterns of variability, the Somaliland clade is characterized by a sufficient mitochondrial haplotype diversity, but low sequence divergence. The population parameters and haplotype networks suggest that the populations belonging to the Somaliland clade probably underwent a recent expansion of its range and population size. It may be explained by a repopulation after the interglacial period providing poor environmental conditions for spiny mice in E and C Somaliland. In contrast, the Djibouti group shows extremely high nucleotide diversity besides that of haplotype one. This suggests a long-term persistence of large and/or structured populations. It may be attributed to a specific history of the Ethiopian Rift and Afar. The results emphasize the importance of the Horn of Africa as a region preserving high endemism.

**Accession Number:** WOS:000545912100001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Frydlova, Petra	P-5008-2016	0000-0001-9385-9743

ISSN: 1616-5047

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**Record 176 of 236**

**Title:** Complex variation in the KLRA (LY49) immunity-related genomic region in horses

**Author(s):** Futas, J (Futas, Jan); Oppelt, J (Oppelt, Jan); Janova, E (Janova, Eva); Musilova, P (Musilova, Petra); Horin, P (Horin, Petr)

**Source:** HLA **Volume:** 96 **Issue:** 3 **Pages:** 257-267 **DOI:** 10.1111/tan.13939 **Early Access Date:** JUL 2020 **Published:** SEP 2020

**Abstract:** Natural killer (NK) cells play important roles in innate and adaptive immunity, as well as in the reproduction of placental mammals. Ly49 (KLRA) molecules represent a lectin-like type of NK cell receptor encoded within a complex genomic region, the NK cell complex. In rodents and horses, an expansion of the genes encoding Ly49 receptors leading to the formation of a gene family was observed. High sequence similarities and frequent high polymorphism of multiple family members represent an obstacle both for their individual identification and for annotation in the reference genomes of their respective species. Here, we focused on resolving complex variation of the KLRA gene family observed in domestic and Przewalski's horses. The KLRA (LY49) genomic region contains six genes (KLRA2-KLRA7) and one putative pseudogene, KLRA1. Two types of polymorphism were observed in the horses analyzed. Copy number variation between haplotypes was documented for the gene KLRA7 by polymerase chain reaction. As expected, the major source of variation of all KLRA genes, including KLRA7, is because of single nucleotide polymorphisms, many of them being nonsynonymous substitutions. Extensive allelic variability of the expanded KLRA (LY49) genes was observed. For four out of the six functional KLRA, high numbers of novel allelic amino acid sequence variants were identified in the genes studied, suggesting that this variation might be of functional importance, especially in the context of high polymorphism of their presumed ligands encoded by major histocompatibility complex class I genes. In fact, polymorphic amino acid sites were mostly found in the ligand-binding C-type lectin-like domain of the putative receptor molecule.

**Accession Number:** WOS:000545706200001

**PubMed ID:** 32421927

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**Record 177 of 236**

**Title:** Lasers in Passive Optical Networks and the Activation Process of an End Unit: A Tutorial

**Author(s):** Horvath, T (Horvath, Tomas); Munster, P (Munster, Petr); Bao, NH (Bao, Ning-Hai)

**Source:** ELECTRONICS **Volume:** 9 **Issue:** 7 **Article Number:** 1114 **DOI:** 10.3390/electronics9071114 **Published:** JUL 2020

**Abstract:** It is 21 years since the first passive optical network (PON) was standardized as an asynchronous transfer mode passive optical network (APON) with same optical distribution network scheme as we know in current networks. A lot of PON networks were standardized in the following years and became an important part of telecommunication. The general principles of these PON networks are described in many papers and books, but only a little information about used lasers is available. The aim of this tutorial is to describe lasers used in PON networks and principles of their operation. The paper describes the principles of single longitudinal mode (SLM), multi longitudinal mode (MLM), distributed-feedback (DFB), and Fabry-Perot (FP) lasers. Furthermore, the lasers are compared by their usage in optical line termination (OLT) for passive optical networks. The second part of this tutorial deals with activation process of optical network unit. The described principle is the same for connection of a new customer or blackout scenario. The end unit is not able to communicate until reach the operational state; each state is defined with physical layer operation and administration and maintenance (PLOAM) messages sequence and their processing.

**Accession Number:** WOS:000554205800001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Munster, Petr	F-6942-2019	0000-0002-4651-8353

eISSN: 2079-9292

**Record 178 of 236**

**Title:** Understanding the rotational variability of K2 targets: HgMn star KIC 250152017 and blue horizontal branch star KIC 249660366?

**Author(s):** Krticka, J (Krticka, J.); Kawka, A (Kawka, A.); Mikulasek, Z (Mikulasek, Z.); Fossati, L (Fossati, L.); Krtickova, I (Krtickova, I.); Prvka, M (Prvka, M.); Janik, J (Janik, J.); Skarka, M (Skarka, M.); Liptaj, R (Liptaj, R.)

**Source:** ASTRONOMY & ASTROPHYSICS **Volume:** 639 **DOI:** 10.1051/0004-6361/202037953 **Published:** JUL 1 2020

**Abstract:** Context. Ultraprecise space photometry enables us to reveal light variability even in stars that were previously deemed constant. A large group of such stars show variations that may be rotationally modulated. This type of light variability is of special interest because it provides precise estimates of rotational rates. Aims. We aim to understand the origin of the light variability of K2 targets that show signatures of rotational modulation. Methods. We used phase-resolved medium-resolution X-shooter spectroscopy to understand the light variability of the stars KIC 250152017 and KIC 249660366, which are possibly rotationally modulated. We determined the atmospheric parameters at individual phases and tested the presence of the rotational modulation in the spectra. Results. KIC 250152017 is a HgMn star, whose light variability is caused by the inhomogeneous surface distribution of manganese and iron. It is only the second HgMn star whose light variability is well understood. KIC 249660366 is a He-weak, high-velocity horizontal branch star with overabundances of silicon and argon. The light variability of this star is likely caused by a reflection effect in this post-common envelope binary.

**Accession Number:** WOS:000547567700008

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kawka, Adela	G-9899-2014	0000-0002-4485-6471

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**Record 179 of 236**

**Title:** Functionalized aromatic esters of the Amaryllidaceae alkaloid haemanthamine and their in vitro and in silico biological activity connected to Alzheimer's disease

**Author(s):** Perinova, R (Perinova, Rozalie); Maafi, N (Maafi, Negar); Korabecny, J (Korabecny, Jan); Kohelova, E (Kohelova, Eliska); De Simone, A (De Simone, Angela); Al Mamun, A (Al Mamun, Abdullah); Hulcova, D (Hulcova, Daniela); Markova, J (Markova, Jana); Kucera, T (Kucera, Tomas); Jun, D (Jun, Daniel); Sافرatova, M (Sافرatova, Marcela); Marikova, J (Marikova, Jana); Andrisano, V (Andrisano, Vincenza); Jenco, J (Jenco, Jaroslav); Kunes, J (Kunes, Jiri); Martinez, A (Martinez, Ana); Novakova, L (Novakova, Lucie); Cahlikova, L (Cahlikova, Lucie)

**Source:** BIOORGANIC CHEMISTRY **Volume:** 100 **Article Number:** 103928 **DOI:** 10.1016/j.bioorg.2020.103928 **Published:** JUL 2020

**Accession Number:** WOS:000540964200009

**PubMed ID:** 32450384

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Maafi, Negar	ABD-1256-2020	0000-0002-4227-7855
Martinez, Ana	L-6414-2014	0000-0002-2707-8110
Jenco, Jaroslav	S-5507-2017	0000-0001-8667-8303

Korabecny, Jan J-6362-2018 0000-0001-6977-7596

ISSN: 0045-2068

eISSN: 1090-2120

**Record 180 of 236****Title:** Convergence verification of the Collatz problem**Author(s):** Barina, D (Barina, David)**Source:** JOURNAL OF SUPERCOMPUTING **DOI:** 10.1007/s11227-020-03368-x **Early Access Date:** JUL 2020**Abstract:** This article presents a new algorithmic approach for computational convergence verification of the Collatz problem. The main contribution of the paper is the replacement of huge precomputed tables containing  $O(2(N))$  entries with small lookup tables comprising just  $O(N)$  elements. Our single-threaded CPU implementation can verify  $4.2 \times 10(9)$  128-bit numbers per second on Intel Xeon Gold 5218 CPU computer, and our parallel OpenCL implementation reaches the speed of  $2.2 \times 10(11)$  128-bit numbers per second on NVIDIA GeForce RTX 2080. Besides the convergence verification, our program also checks for path records during the convergence test.**Accession Number:** WOS:000544846600001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Barina, David A-9035-2015		0000-0003-0917-5512

ISSN: 0920-8542

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**Record 181 of 236****Title:** Microwave spectroscopy of planar and quasi-planar organic molecules: Indole and 1,2,3,4-tetrahydroquinoline**Author(s):** Nesvadba, R (Nesvadba, Radim); Vavra, K (Vavra, Karel); Lukova, K (Lukova, Katerina); Kania, P (Kania, Patrik); Koucky, J (Koucky, Jan); Urban, S (Urban, Stepan)**Source:** JOURNAL OF QUANTITATIVE SPECTROSCOPY & RADIATIVE TRANSFER **Volume:** 249 **Article Number:** 107033 **DOI:** 10.1016/j.jqsrt.2020.107033 **Published:** JUL 2020**Abstract:** In this study, 3179 and 3813 rotational transition frequencies for indole and 1,2,3,4-tetrahydroquinoline, respectively, were analyzed using the PGOPHER software. In both analyses, all the matrix elements of the sextic rotational Hamiltonians were fitted simultaneously to the hyperfine quadrupole terms. The global fits of all the transition frequencies provided the most precise ground state molecular parameters for both molecules, so far. The presented experimental results are in concordance with the density functional theory calculations. (C) 2020 Elsevier Ltd. All rights reserved.**Accession Number:** WOS:000542287900006**Conference Title:** 19th Symposium on High Resolution Molecular Spectroscopy (HighRus)**Conference Date:** JUL 01-05, 2019**Conference Location:** Nizhny Novgorod, RUSSIA**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kania, Patrik	C-5386-2012	0000-0001-8338-3569
Koucky, Jan	G-7512-2019	
Nesvadba, Radim		0000-0003-1506-6195
Koucky, Jan		0000-0001-9498-9400

ISSN: 0022-4073

eISSN: 1879-1352

**Record 182 of 236****Title:** Molecular dynamics simulations of singlet oxygen atoms reactions with water leading to hydrogen peroxide**Author(s):** Xu, SF (Xu, Shaofeng); Jirasek, V (Jirasek, Vit); Lukes, P (Lukes, Petr)**Source:** JOURNAL OF PHYSICS D-APPLIED PHYSICS **Volume:** 53 **Issue:** 27 **Article Number:** 275204 **DOI:** 10.1088/1361-6463/ab8321 **Published:** JUL 1 2020**Abstract:** The formation mechanisms of hydrogen peroxide due to the interaction of oxygen atom from the cold atmospheric plasmas in contact with water are not fully understood. Previous work on molecular dynamics (MD) simulations of interactions of O atoms in bulk water based on reactive force field and density-functional tight-binding method did not observe the formation of  $H_2O_2$ . We used  $H_2O_2$ -O system to explore the reaction mechanisms for atomic oxygen radical in water. Our calculations revealed that triplet (ground) state oxygen was not reactive. Oxywater-similar structure O-OH<sub>2</sub>-OH-H<sub>3</sub>O<sup>+</sup> were formed. In most of simulated cases, hydrogen peroxide was observed as a final product. The formation pathways of hydrogen peroxide exhibited large complexities for the simple hydrogen bonded system. According to the sources and pathways of the hydrogen atom being bonded in hydrogen peroxide molecule, mechanisms can be classified into (1) hydrogen-abstraction, (2) hydrogen-transfer n (n = 3, 4, 5, 6, 7, 8), (3) proton-delivery n = 2, 3, (4) proton-transfer. It was confirmed that for correct prediction of reaction mechanisms is better to use quantum molecular dynamic simulations.**Accession Number:** WOS:000536020000001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lukes, Petr	G-2712-2014	0000-0002-7330-0456

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eISSN: 1361-6463

**Record 183 of 236****Title:** Primordial mass segregation of star clusters with primordial binaries**Author(s):** Pavlik, V (Pavlik, Vaclav)**Source:** ASTRONOMY & ASTROPHYSICS **Volume:** 638 **Article Number:** A155 **DOI:** 10.1051/0004-6361/202037490 **Published:** JUN 29 2020**Abstract:** Context. Observations of young star-forming regions suggest that star clusters are born completely mass segregated. These initial conditions are, however, gradually lost as the star cluster evolves dynamically. For star clusters with single stars only and a canonical initial mass function, it has been suggested that traces of these initial conditions vanish at a time  $\tau(v)$  between 3 and 3.5 t(rh) (initial half-mass relaxation times). Aims. Since a significant fraction of stars are observed in binary systems and it is widely accepted that most stars are born in binary systems, we aim to investigate what role a primordial binary population (even up to 100% binaries) plays in the loss of primordial mass segregation of young star clusters. Methods. We used numerical N-body models similar in size to the Orion Nebula Cluster (ONC) - a representative of young open clusters - integrated over several relaxation times to draw conclusions on the evolution of its mass segregation. We also compared our models to the observed ONC. Results. We found that  $\tau(v)$  depends on the binary star fraction and the distribution of initial binary parameters that include a semi-major axis, eccentricity, and mass ratio. For instance, in the models with 50% binaries, we find  $\tau(v) = (2.7 \pm 0.8)$  t(rh), while for 100% binary fraction, we find a lower value  $\tau(v) = (2.1 \pm 0.6)$  t(rh). We also conclude that the initially completely mass segregated clusters, even with binaries, are more compatible with the present-day ONC than the non-segregated ones.**Accession Number:** WOS:000549956900004**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pavlik, Vaclav C-8848-2017		0000-0002-3031-062X

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eISSN: 1432-0746

**Record 184 of 236****Title:** Yeast Spt6 Reads Multiple Phosphorylation Patterns of RNA Polymerase II C-Terminal Domain In Vitro**Author(s):** Brazda, P (Brazda, Pavel); Krejciikova, M (Krejciikova, Magdalena); Kasiliauskaite, A (Kasiliauskaite, Aiste); Smirakova, E (Smirakova, Eliska); Klumpler, T (Klumpler, Tomas); Vacha, R (Vacha, Robert); Kubicek, K (Kubicek, Karel); Stefl, R (Stefl, Richard)**Source:** JOURNAL OF MOLECULAR BIOLOGY **Volume:** 432 **Issue:** 14 **Pages:** 4092-4107 **DOI:** 10.1016/j.jmb.2020.05.007 **Published:** JUN 26 2020

**Abstract:** Transcription elongation factor Spt6 associates with RNA polymerase II (RNAP II) via a tandem SH2 (tSH2) domain. The mechanism and significance of the RNAP II-Spt6 interaction is still unclear. Recently, it was proposed that Spt6-tSH2 is recruited via a newly described phosphorylated linker between the Rpb1 core and its C-terminal domain (CTD). Here, we report binding studies with isolated tSH2 of Spt6 (Spt6-tSH2) and Spt6 lacking the first unstructured 297 residues (Spt6AN) with a minimal CTD substrate of two repetitive heptads phosphorylated at different sites. The data demonstrate that Spt6 also binds the phosphorylated CTD, a site that was originally proposed as a recognition epitope. We also show that an extended CTD substrate harboring 13 repetitive heptads of the tyrosine-phosphorylated CTD binds Spt6-tSH2 and Spt6AN with tighter affinity than the minimal CTD substrate. The enhanced binding is achieved by avidity originating from multiple phosphorylation marks present in the CTD. Interestingly, we found that the steric effects of additional domains in the Spt6AN construct partially obscure the binding of the tSH2 domain to the multivalent ligand. We show that Spt6-tSH2 binds various phosphorylation patterns in the CTD and found that the studied combinations of phospho-CTD marks (1,2; 1,5; 2,4; and 2,7) all facilitate the interaction of CTD with Spt6. Our structural studies reveal a plasticity of the tSH2 binding pockets that enables the accommodation of CTDs with phosphorylation marks in different registers. (C) 2020 The Authors. Published by Elsevier Ltd.

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**PubMed ID:** 32439331

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#### Record 185 of 236

**Title:** Longitudinally monitored lifetime changes in blood heavy metal concentrations and their health effects in urban birds

**Author(s):** Bauerova, P (Bauerova, Petra); Krajcingrova, T (Krajcingrova, Tereza); Tesicky, M (Tesicky, Martin); Velova, H (Velova, Hana); Hranicek, J (Hranicek, Jakub); Musil, S (Musil, Stanislav); Svobodova, J (Svobodova, Jana); Albrecht, T (Albrecht, Tomas); Vinkler, M (Vinkler, Michal)

**Source:** SCIENCE OF THE TOTAL ENVIRONMENT **Volume:** 723 **Article Number:** 138002 **DOI:** 10.1016/j.scitotenv.2020.138002 **Published:** JUN 25 2020

**Abstract:** Urban heavy metal pollution can impair the health of humans and other organisms inhabiting cities. While birds are suggested as one of the appropriate bioindicators for essential and non-essential trace element monitoring, the process of particular elements' accumulation in blood and its possible adverse health effects during ageing of individuals remain unexplored. We have investigated lifetime changes in blood lead (Pb), cadmium (Cd), arsenic (As) and zinc (Zn) concentrations and searched for links to health-related traits in sub-urban free-living great tit (*Parus major*) population monitored over a long period of time. The blood As concentrations were under the limit of detection in most samples. The blood Pb levels showed a non-linear relationship to individuals age, where the highest Pb concentrations were measured in nestlings and in a very small group of highly senescent birds (over 7 years old), while no clear trend was observed for the majority of the adult age stages. No age-related patterns were found for blood Cd or Zn concentrations. The positive relationship between date of capture and blood Cd and Zn levels may reflect seasonal changes in diet composition. We did not reveal any anaemia-like conditions (decreased total erythrocyte count or increased immature erythrocyte count) in relation to blood heavy metal concentrations in the investigated birds. Total leukocyte counts, heterophil/lymphocyte (H/L) ratio and total heterophil and lymphocyte counts increased with increasing Pb, Cd and Zn concentrations in blood. This study demonstrates the suitability of avian blood for actual heavy metal spatial and temporal biomonitoring even in situations when the precise age of the individuals remains unknown. (C) 2020 Elsevier B.V. All rights reserved.

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**PubMed ID:** 32213411

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Svobodova, Jana	G-9692-2012	0000-0001-6161-4899
Vinkler, Michal	G-2072-2011	0000-0003-3572-9494
Musil, Stanislav	N-7751-2013	0000-0001-8003-0370
Albrecht, Tomas	A-1130-2011	
Tesicky, Martin	L-3370-2017	0000-0001-8097-5331

**ISSN:** 0048-9697

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#### Record 186 of 236

**Title:** Laser capture microdissection in combination with mass spectrometry: Approach to characterization of tissue-specific proteomes of *Eudiplozoon nipponicum* (Monogenea, Polyopisthocotylea)

**Author(s):** Roudnický, P (Roudnický, Pavel); Patesil, D (Patesil, David); Zdrahal, Z (Zdrahal, Zbynek); Gelnar, M (Gelnar, Milan); Kasny, M (Kasny, Martin)

**Source:** PLOS ONE **Volume:** 15 **Issue:** 6 **Article Number:** e0231681 **DOI:** 10.1371/journal.pone.0231681 **Published:** JUN 17 2020

**Abstract:** *Eudiplozoon nipponicum* (Goto, 1891) is a hematophagous monogenean ectoparasite which inhabits the gills of the common carp (*Cyprinus carpio*). Heavy infestation can lead to anemia and in conjunction with secondary bacterial infections cause poor health and eventual death of the host. This study is based on an innovative approach to protein localization which has never been used in parasitology before. Using laser capture microdissection, we dissected particular areas of the parasite body without contaminating the samples by surrounding tissue and in combination with analysis by mass spectrometry obtained tissue-specific proteomes of tegument, intestine, and parenchyma of our model organism, *E. nipponicum*. We successfully verified the presence of certain functional proteins (e.g. cathepsin L) in tissues where their presence was expected (intestine) and confirmed that there were no traces of these proteins in other tissues (tegument and parenchyma). Additionally, we identified a total of 2,059 proteins, including 72 peptidases and 33 peptidase inhibitors. As expected, the greatest variety was found in the intestine and the lowest variety in the parenchyma. Our results are significant on two levels. Firstly, we demonstrated that one can localize all proteins in one analysis and without using laboratory animals (antibodies for immunolocalization of single proteins). Secondly, this study offers the first complex proteomic data on not only the *E. nipponicum* but within the whole class of Monogenea, which was from this point of view until recently neglected.

**Accession Number:** WOS:000542759600012

**PubMed ID:** 32555742

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Roudnický, Pavel		0000-0002-6904-7646

**ISSN:** 1932-6203

#### Record 187 of 236

**Title:** Comparative analyses of DNA repeats and identification of a novel Fesreba centromeric element in fescues and ryegrasses

**Author(s):** Zwyratkova, J (Zwyratkova, Jana); Nemeckova, A (Nemeckova, Alzbeta); Cizkova, J (Cizkova, Jana); Holusova, K (Holusova, Katerina); Kapustova, V (Kapustova, Veronika); Svacina, R (Svacina, Radim); Kopecky, D (Kopecky, David); Till, BJ (Till, Bradley John); Dolezel, J (Dolezel, Jaroslav); Hribova, E (Hribova, Eva)

**Source:** BMC PLANT BIOLOGY **Volume:** 20 **Issue:** 1 **Article Number:** 280 **DOI:** 10.1186/s12870-020-02495-0 **Published:** JUN 17 2020

**Abstract:** Background Cultivated grasses are an important source of food for domestic animals worldwide. Increased knowledge of their genomes can speed up the development of new cultivars with better quality and greater resistance to biotic and abiotic stresses. The most widely grown grasses are tetraploid ryegrass species (*Lolium*) and diploid and hexaploid fescue species (*Festuca*). In this work, we characterized repetitive DNA sequences and their contribution to genome size in five fescue and two ryegrass species as well as one fescue and two ryegrass cultivars. Results Partial genome sequences produced by Illumina sequencing technology were used for genome-wide comparative analyses with the RepeatExplorer pipeline. Retrotransposons were the most abundant repeat type in all seven grass species. The Athalia element of the Ty3/gypsy family showed the most striking differences in copy number between fescues and ryegrasses. The sequence data enabled the assembly of the long terminal repeat (LTR) element Fesreba, which is highly enriched in centromeric and (peri)centromeric regions in all species. A combination of fluorescence in situ hybridization (FISH) with a probe specific to the Fesreba element and immunostaining with centromeric histone H3 (CENH3) antibody showed their co-localization and indicated a possible role of Fesreba in centromere function. Conclusions Comparative repeatome analyses in a set of fescues and ryegrasses provided new insights into their genome organization and divergence, including the assembly of the LTR element Fesreba. A new LTR element Fesreba was identified and found in abundance in centromeric regions of the fescues and ryegrasses. It may play a role in the function of their centromeres.

**Accession Number:** WOS:000542955600020

**PubMed ID:** 32552738

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Dolezel, Jaroslav	B-7716-2008	0000-0002-6263-0492
Cizkova, Jana		0000-0001-7787-1849
Holusova, Katerina	F-7694-2014	0000-0002-4531-7170
Zwyratkova, Jana		0000-0002-9721-1386
Hribova, Eva		0000-0002-6868-4344



ISSN: 1471-2229

## Record 188 of 236

**Title:** Evolution of multiple sex-chromosomes associated with dynamic genome reshuffling in Leptidea wood-white butterflies**Author(s):** Yoshido, A (Yoshido, Atsuo); Sichova, J (Sichova, Jindra); Pospisilov, K (Pospisilov, Kristyna); Nguyen, P (Nguyen, Petr); Volenikov, A (Volenikov, Anna); Safar, J (Safar, Jan); Provaznik, J (Provaznik, Jan); Vila, R (Vila, Roger); Marec, F (Marec, Frantisek)**Source:** HEREDITY Volume: 125 Issue: 3 Pages: 138-154 DOI: 10.1038/s41437-020-0325-9 Early Access Date: JUN 2020 Published: SEP 2020**Abstract:** Sex-chromosome systems tend to be highly conserved and knowledge about their evolution typically comes from macroevolutionary inference. Rapidly evolving complex sex-chromosome systems represent a rare opportunity to study the mechanisms of sex-chromosome evolution at unprecedented resolution. Three cryptic species of wood-white butterflies—*Leptidea juvernica*, *L. sinapis* and *L. reali*—have each a unique set of multiple sex-chromosomes with 3-4 W and 3-4 Z chromosomes. Using a transcriptome-based microarray for comparative genomic hybridisation (CGH) and a library of bacterial artificial chromosome (BAC) clones, both developed in *L. juvernica*, we identified Z-linked orthologs of *Bombus* morigenes and mapped them by fluorescence in situ hybridisation (FISH) with BAC probes on multiple Z chromosomes. In all three species, we determined synteny blocks of autosomal origin and reconstructed the evolution of multiple sex-chromosomes. In addition, we identified W homologues of Z-linked orthologs and characterised their molecular differentiation. Our results suggest that the multiple sex-chromosome system evolved in a common ancestor as a result of dynamic genome reshuffling through repeated rearrangements between the sex chromosomes and autosomes, including translocations, fusions and fissions. Thus, the initial formation of neo-sex chromosomes could not have played a role in reproductive isolation between these *Leptidea* species. However, the subsequent species-specific fissions of several neo-sex chromosomes could have contributed to their reproductive isolation. Then, significantly increased numbers of Z-linked genes and independent neo-W chromosome degeneration could accelerate the accumulation of genetic incompatibilities between populations and promote their divergence resulting in speciation.**Accession Number:** WOS:000539670600001**PubMed ID:** 32518391**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Pospisilova, Kristyna	AAC-3036-2021	
Nguyen, Petr	AAI-5203-2020	0000-0003-1395-4287
Marec, Frantisek	G-7943-2014	0000-0002-6745-5603
Pospisilova, Kristyna		0000-0001-9426-9411
Vila, Roger	A-1817-2012	0000-0002-2447-4388
Yoshido, Atsuo		0000-0003-0343-2709
Volenikova, Anna		0000-0002-9504-8044

ISSN: 0018-067X

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## Record 189 of 236

**Title:** Surprisingly broad applicability of the cc-pVnZ-F12 basis set for ground and excited states**Author(s):** Kruse, H (Kruse, Holger); Szabla, R (Szabla, Rafal); Sponer, J (Sponer, Jiri)**Source:** JOURNAL OF CHEMICAL PHYSICS Volume: 152 Issue: 21 DOI: 10.1063/5.0006871 Published: JUN 7 2020**Abstract:** Excellent convergence properties for the (aug)-cc-pVnZ-F12 basis set family, purpose-made for explicitly correlated calculations, are demonstrated with conventional wave function methods and Kohn-Sham density functional theory for various ground and excited-state calculations. Among the ground-state properties studied are dipole moments, covalent bond lengths, and interaction and reaction energies. For excited states, we looked at vertical excitation energies, UV absorption, and excited-state absorption spectra. Convergence is compared against the basis sets cc-pVnZ, def2-nVD, aug-pcseg-n, and nZaPa-NR. It is established that the cc-pVnZ-F12 family consistently yields results of  $n + 1$  quality and better. Especially, the cc-pVDZ-F12 basis set is found to be a basis set of good cost vs performance trade-off.**Accession Number:** WOS:000538149300001**PubMed ID:** 32505162**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kruse, Holger	D-3615-2009	0000-0002-0560-1513
Szabla, Rafal	A-6910-2013	0000-0002-1668-8044

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## Record 190 of 236

**Title:** Stereoselective Bromoboration of Acetylene with Boron Tribromide: Preparation and Cross-Coupling Reactions of (Z)-Bromovinylboronates**Author(s):** Polasek, J (Polasek, Jan); Paciorek, J (Paciorek, Jan); Stosek, J (Stosek, Jakub); Semrad, H (Semrad, Hugo); Munzarova, M (Munzarova, Marketa); Mazal, C (Mazal, Ctibor)**Source:** JOURNAL OF ORGANIC CHEMISTRY Volume: 85 Issue: 11 Pages: 6992-7000 DOI: 10.1021/acs.joc.0c00341 Published: JUN 5 2020**Abstract:** The mechanism of acetylene bromoboration in neat boron tribromide was studied carefully by means of experiment and theory. Besides the syn-addition mechanism through a four-center transition state, radical and polar anti-addition mechanisms are postulated, both triggered by HBr, which is evidenced also to take part in the Z/E isomerization of the product. The proposed mechanism is well supported by ab initio calculations at the MP2/6-31+G\* level with Ahlrichs' SVP all-electron basis for Br. Implicit solvation in CH<sub>2</sub>Cl<sub>2</sub> has been included using the PCM and/or SMD continuum solvent models. Comparative case studies have been performed involving the B3LYP/6-31+G\* with Ahlrichs' SVP for Br and MP2/Def2TZVPP levels. The mechanistic studies resulted in development of a procedure for stereoselective bromoboration of acetylene yielding E/Z mixtures of dibromo(bromovinyl)borane with the Z-isomer as a major product (up to 85%). Transformation to the corresponding pinacol and neopentyl glycol boronates and stereoselective decomposition of their E-isomer provided pure (Z)-(2-bromovinyl)boronates in 57-60% overall yield. Their reactivity in a Negishi cross-coupling reaction was tested. An example of the one-pot reaction sequence of Negishi and Suzuki-Miyaura cross-couplings for synthesis of combretastatin A4 is also presented.**Accession Number:** WOS:000538764000016**PubMed ID:** 32436705**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Polasek, Jan		0000-0001-7153-8666

ISSN: 0022-3263

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## Record 191 of 236

**Title:** FlexAlign: An Accurate and Fast Algorithm for Movie Alignment in Cryo-Electron Microscopy**Author(s):** Strelak, D (Strelak, David); Filipovic, J (Filipovic, Jiri); Jimenez-Moreno, A (Jimenez-Moreno, Amaya); Carazo, JM (Carazo, Jose Maria); Sorzano, COS (Sorzano, Carlos Oscar S.)**Source:** ELECTRONICS Volume: 9 Issue: 6 Article Number: 1040 DOI: 10.3390/electronics9061040 Published: JUN 2020**Abstract:** Cryogenic Electron Microscopy (Cryo-EM) has been established as one of the key players in Structural Biology. It can reconstruct a 3D model of the sample at the near-atomic resolution, which led to a Method of the Year award by Nature, and the Nobel Prize in 2017. With the growing number of facilities, faster microscopes, and new imaging techniques, new algorithms are needed to process the so-called movies data produced by the microscopes in real-time, while preserving a high resolution and maximum of additional information. In this article, we present a new algorithm used for movie alignment, called FlexAlign. FlexAlign is able to correctly compensate for the shift produced during the movie acquisition on-the-fly, using the current generation of hardware. The algorithm performs a global and elastic local registration of the movie frames using Cross-Correlation and B-spline interpolation for high precision. We show that our execution time is compatible with real-time correction and that we preserve the high-resolution information up to high frequency.**Accession Number:** WOS:000551113800001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Filipovic, Jiri	H-4311-2013	0000-0002-5703-9673

Jimenez-Moreno, Amaya AAA-7450-2021	
S. Sorzano, Carlos Oscar F-2639-2016	0000-0002-9473-283X
eISSN: 2079-9292	

**Record 192 of 236**

**Title:** Nonlinear reflection as a cause of the short-latency component in stimulus-frequency otoacoustic emissions simulated by the methods of compression and suppression

**Author(s):** Vencovsky, V (Vencovsky, Vaclav); Vetesnik, A (Vetesnik, Ales); Gummer, AW (Gummer, Anthony W.)

**Source:** JOURNAL OF THE ACOUSTICAL SOCIETY OF AMERICA **Volume:** 147 **Issue:** 6 **Pages:** 3992-4008 **DOI:** 10.1121/10.0001394 **Published:** JUN 2020

**Abstract:** Stimulus-frequency otoacoustic emissions (SFOAEs) are generated by coherent reflection of forward traveling waves by perturbations along the basilar membrane. The strongest wavelets are backscattered near the place where the traveling wave reaches its maximal amplitude (tonotopic place). Therefore, the SFOAE group delay might be expected to be twice the group delay estimated in the cochlear filters. However, experimental data have yielded steady-state SFOAE components with near-zero latency. A cochlear model is used to show that short-latency SFOAE components can be generated due to nonlinear reflection of the compressor or suppressor tones used in SFOAE measurements. The simulations indicate that suppressors produce more pronounced short-latency components than compressors. The existence of nonlinear reflection components due to suppressors can also explain why SFOAEs can still be detected when suppressors are presented more than half an octave above the probe-tone frequency. Simulations of the SFOAE suppression tuning curves showed that phase changes in the SFOAE residual as the suppressor frequency increases are mostly determined by phase changes of the nonlinear reflection component.

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**PubMed ID:** 32611132

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Vencovsky, Vaclav		0000-0002-5556-0924

ISSN: 0001-4966

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**Record 193 of 236**

**Title:** Dataset of molecular dynamics simulation trajectories of amino-acid solutions with various force fields, water models and modified force field parameters

**Author(s):** Prusa, J (Prusa, Jiri); Cifra, M (Cifra, Michal)

**Source:** DATA IN BRIEF **Volume:** 30 **Article Number:** 105483 **DOI:** 10.1016/j.dib.2020.105483 **Published:** JUN 2020

**Abstract:** We present molecular dynamics (MD) trajectories of water solutions of eight zwitterionic amino-acids (L-form) glycine (GLY), alanine (ALA), proline (PRO), threonine (THR), leucine (LEU), glutamine (GLN), histidine (HIS) and tyrosine (TYR) using various force field (OPLS-AA, Amber99ff-SB, GROMOS96 54a7, CHARMM19) and water model (SPC/E, TIP3P) combinations. Additionally, we present OPLS-AA molecular dynamics (MD) trajectories for alanine (ALA), leucine (LEU), glutamine (GLN), and tyrosine (TYR) varying the values of major force field parameters: charge on all amino acid atoms, bond length (all amino acid bonds), Lennard-Jones potential epsilon parameter and stiffness of bond angles. Our data enable to uncover sensitivity of molecular dynamics derived analysis to variation of force field and water models and force field parameters. This data set was used to understand the effect of molecular dynamics parameters on dielectric properties of amino acid solutions [1]. (C) 2020 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license. (<http://creativecommons.org/licenses/by/4.0/>)

**Accession Number:** WOS:000542612000019

**PubMed ID:** 32368577

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Cifra, Michal	D-4416-2013	0000-0002-8853-9523

ISSN: 2352-3409

**Record 194 of 236**

**Title:** Expansion of Hot Plasma with Kappa Distribution into Cold Plasma

**Author(s):** Benacek, J (Benacek, Jan); Karlicky, M (Karlicky, Marian)

**Source:** ASTROPHYSICAL JOURNAL **Volume:** 896 **Issue:** 1 **Article Number:** 9 **DOI:** 10.3847/1538-4357/ab89a5 **Published:** JUN 2020

**Abstract:** The X-ray emission of coronal flare sources can be explained by considering the kappa electron distribution. Motivated by this fact, we study the problem of how hot plasma with the kappa distribution of electrons is confined in these sources. For comparison, we analyze the same problem, but with the Maxwellian distribution. We use a 3D particle-in-cell code, which is large in one direction and thus effectively only one-dimensional, but describe all electromagnetic effects. In the case with the Maxwellian distribution, and in agreement with the previous studies, we show a formation of the double layer at the hot-cold transition region that suppresses the flux of hot electrons from hot plasma into the cold one. In the case with the kappa distribution, contrary to the Maxwellian case, we found that there are several fronts with the double layers in the hot-cold transition region. It is caused by a more extended tail in the kappa case than in the Maxwellian one. The electrons from the extended tail freely escape from the hot plasma into a cold one. They form a beam that generates the return current and also Langmuir turbulence, where Langmuir waves accumulated at some locations. At these locations, owing to the ponderomotive force, Langmuir waves generate density depressions, where the double layers with the thermal fronts that suppress the hot electron flux, are formed. We also show how protons accelerate in these processes. Finally, we compare the Kappa and Maxwellian cases and discuss how these processes could be observed.

**Accession Number:** WOS:000540822700001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Karlicky, Marian	G-9023-2014	0000-0002-3963-8701
Benacek, Jan	C-9189-2019	0000-0002-4319-8083

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**Record 195 of 236**

**Title:** Smart Grids Data Analysis: A Systematic Mapping Study

**Author(s):** Rossi, B (Rossi, Bruno); Chren, S (Chren, Stanislav)

**Source:** IEEE TRANSACTIONS ON INDUSTRIAL INFORMATICS **Volume:** 16 **Issue:** 6 **Pages:** 3619-3639 **DOI:** 10.1109/TII.2019.2954098 **Published:** JUN 2020

**Abstract:** Data analytics and data science play a significant role in nowadays society. In the context of smart grids, the collection of vast amounts of data has seen the emergence of a plethora of data analysis approaches. In this article, we conduct a systematic mapping study aimed at getting insights about different facets of SG data analysis: application subdomains (e.g., power load control), aspects covered (e.g., forecasting), used techniques (e.g., clustering), tool support, research methods (e.g., experiments/simulations), and replicability/reproducibility of research. The final goal is to provide a view of the current status of research. Overall, we found that each subdomain has its peculiarities in terms of techniques, approaches, and research methodologies applied. Simulations and experiments play a crucial role in many areas. The replicability of studies is limited concerning the provided implemented algorithms, and to a lower extent due to the usage of private datasets.

**Accession Number:** WOS:000526381800001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Rossi, Bruno		0000-0002-8659-1520
Chren, Stanislav		0000-0002-6675-8119

ISSN: 1551-3203

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**Record 196 of 236**

**Title:** Raman Optical Activity of Glucose and Sorbose in Extended Wavenumber Range

**Author(s):** Palivec, V (Palivec, Vladimir); Michal, P (Michal, Pavel); Kapitan, J (Kapitan, Josef); Martinez-Seara, H (Martinez-Seara, Hector); Bour, P (Bour, Petr)

**Source:** CHEMPHYSICHEM **Volume:** 21 **Issue:** 12 **Pages:** 1272-1279 **DOI:** 10.1002/cphc.202000261 **Early Access Date:** MAY 2020 **Published:** JUN 16 2020

**Abstract:** Raman optical activity (ROA) is pursued as a promising method for structural analyses of sugars in aqueous solutions. In the present study, experimental Raman and ROA spectra of glucose and sorbose obtained in an extended range (50–4000 cm<sup>-1</sup>) are interpreted using molecular dynamics and density functional theory, with the emphasis on CH stretching modes. A reasonable theoretical basis for spectral interpretation was obtained already at the harmonic level. Anharmonic corrections led to minor shifts of band positions (up to 25 cm<sup>-1</sup>) below 2000 cm<sup>-1</sup>, while the CH stretching bands shifted more, by similar to 180 cm<sup>-1</sup>, and better reproduced the experiment. However, the anharmonicities could be included on a relatively low approximation level only, and they did not always improve the harmonic band shapes. The dependence on the structure and conformation shows that the CH stretching ROA spectral pattern is a sensitive marker useful in saccharide structure studies.

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**PubMed ID:** 32337784

**ISSN:** 1439-4235

**eISSN:** 1439-7641

#### Record 197 of 236

**Title:** Finite Systems under Pressure: Assessing Volume Definition Models from Parallel-Tempering Monte Carlo Simulations

**Author(s):** Vitek, A (Vitek, Ales); Arismendi-Arrieta, DJ (Arismendi-Arrieta, Daniel J.); Sarmanova, M (Sarmanova, Martina); Kalus, R (Kalus, Rene); Prosmi, R (Prosmi, Rita)

**Source:** JOURNAL OF PHYSICAL CHEMISTRY A **Volume:** 124 **Issue:** 20 **Pages:** 4036-4047 **DOI:** 10.1021/acs.jpca.0c00881 **Published:** MAY 21 2020

**Abstract:** We have investigated different approaches to handling parallel-tempering Monte Carlo (PTMC) simulations in the isothermal-isobaric ensemble of molecular cluster/nanoparticle systems for predicting structural phase diagram transitions. We have implemented various methodologies that consist of treating pressure implicitly through its effect on the volume. Thus, the main problem in the simulations under nonzero pressure becomes the volume definition of the finite nonperiodic system, and we considered approaches based on the particles' coordinates. Various volume models, namely container-volume, particle-volume, average-volume, ellipsoids-volume, and convex hull-volume, were employed, and the required corrections for each of them in the Monte Carlo computations were introduced. Finally, we explored the effects of volume/pressure changes for all models on structural phase transitions of a test system, such as the small "icelike" (H<sub>2</sub>O)(12) water cluster. The temperature and pressure dependence of the cluster's heat capacity and energy-volume Pearson correlation coefficient were studied, phase diagrams were constructed using a multiple-histogram method, and attempts were made to identify phase transitions to particular cluster structures. Our results show significant differences between the employed volume models, and we discuss all pressure-induced, such as solid-solid-, solid-liquid-, and liquid-gas-like, phase transformations in the present study.

**Accession Number:** WOS:000537424600008

**PubMed ID:** 32370498

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Arrieta, Daniel J. Arismendi	H-9113-2013	0000-0002-4917-2466
Prosmi, Rita		0000-0002-1557-1549
Sarmanova, Martina		0000-0003-4080-4145

**ISSN:** 1089-5639

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#### Record 198 of 236

**Title:** Tracing the early steps of competition-driven eco-morphological divergence in two sister species of passerines

**Author(s):** Sottas, C (Sottas, Camille); Reif, J (Reif, Jiri); Kreisinger, J (Kreisinger, Jakub); Schmiedova, L (Schmiedova, Lucie); Sam, K (Sam, Katerina); Osiejuk, TS (Osiejuk, Tomasz S.); Reifova, R (Reifova, Radka)

**Source:** EVOLUTIONARY ECOLOGY **Volume:** 34 **Issue:** 4 **Pages:** 501-524 **DOI:** 10.1007/s10682-020-10050-4 **Early Access Date:** MAY 2020 **Published:** AUG 2020

**Abstract:** Competition-driven feeding niche separation is assumed to be an important driver of the morphological divergence of co-occurring animal species. However, despite a strong theoretical background, empirical studies showing a direct link between competition, diet divergence and specific morphological adaptations are still scarce. Here we studied the early steps of competition-driven eco-morphological divergence in two closely related passerines: the common nightingale (*Luscinia megarhynchos*) and the thrush nightingale (*Luscinia luscinia*). Our aim was to test whether previously-observed divergence in bill morphology and habitat in sympatric populations of both species is associated with dietary niche divergence. We collected and analysed data on (1) diet, using both DNA metabarcoding and visual identification of prey items, (2) habitat use, and (3) bill morphology in sympatric populations of both nightingale species. We tested whether the species differ in diet composition and whether there are any associations among diet, bill morphology and habitat use. We found that the two nightingale species have partitioned their feeding niches, and showed that differences in diet may be partially associated with the divergence in bill length in sympatric populations. We also observed an association between bill length and habitat use, suggesting that competition-driven habitat segregation could be linked with dietary and bill size divergence. Our results suggest that interspecific competition is an important driver of species' eco-morphological divergence after their secondary contact, and provide insight into the early steps of such divergence in two closely related passerine species. Such divergence may facilitate species coexistence and strengthen reproductive isolation between species, and thus help to complete the speciation process.

**Accession Number:** WOS:000533198000001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kreisinger, Jakub	H-4020-2011	
Schmiedova, Lucie	S-3351-2017	0000-0003-2180-5281
Schmiedova, Lucie	AAX-8167-2020	0000-0003-2180-5281
Sam, Katerina	I-2209-2014	0000-0002-3436-0579
Reif, Jiri	I-9168-2017	0000-0003-2553-7333
Osiejuk, Tomasz		0000-0001-5980-7421

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#### Record 199 of 236

**Title:** Multiplication Algorithm Based on Collatz Function

**Author(s):** Barina, D (Barina, David)

**Source:** THEORY OF COMPUTING SYSTEMS **Volume:** 64 **Issue:** 8 **Pages:** 1331-1337 **DOI:** 10.1007/s00224-020-09986-5 **Early Access Date:** MAY 2020 **Published:** NOV 2020

**Abstract:** This article presents a new multiplication algorithm based on the Collatz function. Assuming the validity of the Collatz conjecture, the time complexity of multiplying two  $n$ -digit numbers is  $O(kn)$ , where the  $k$  is the number of odd steps in the Collatz trajectory of the first multiplicand. Most likely, the algorithm is only of theoretical interest.

**Accession Number:** WOS:000533052700001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Barina, David	A-9035-2015	0000-0003-0917-5512

**ISSN:** 1432-4350

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#### Record 200 of 236

**Title:** Electrochemical and spectroscopic study of 2-iodobenzoic acid and 2-iodosobenzoic acid anodic oxidation in aqueous environment

**Author(s):** Devadas, B (Devadas, Balamurugan); Svoboda, J (Svoboda, Jan); Krupicka, M (Krupicka, Martin); Bystron, T (Bystron, Tomas)

**Source:** ELECTROCHIMICA ACTA **Volume:** 342 **Article Number:** 136080 **DOI:** 10.1016/j.electacta.2020.136080 **Published:** MAY 10 2020

**Abstract:** 2-iodosobenzoic acid and especially IBX represent interesting selective and green hypervalent iodine oxidants. Mainly due to issues connected with their preparation, use of these compounds is limited to laboratory scale. From this point of view, the electrochemical synthesis represents interesting platform for inherently safer production of these highly valued oxidants. In order to provoke and allow more intense investigation in this direction, this work aimed to present basic aspects of electrochemical behaviour of these compounds in aqueous environment using several anode materials. A combination of various experimental approaches in combination with time-dependent density functional theory calculations allowed determining compounds speciation in a wide range of pH values. The most interesting in this sense is iodoxol ring opening after/during deprotonation of 2-iodosobenzoic acid to 2-iodosobenzoate. This process is accompanied by addition of water molecule to the iodine atom. Using voltammetry and controlled potential preparative batch electrolysis allowed constructing approximate form of Pourbaix diagram of the investigated compounds. Finally, diffusion coefficients of investigated compounds and anodic charge transfer coefficients of oxidation reactions were determined based on detailed analysis of linear voltammograms. The results provide a solid base for further investigation of



electrochemical synthesis of 2-iodosobenzoic acid and IBX in aqueous environment. (C) 2020 Elsevier Ltd. All rights reserved.

**Accession Number:** WOS:000524987200012

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Krupicka, Martin A	1810-2009	0000-0002-9132-5825
Svoboda, Jan		0000-0003-4297-448X

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**Record 201 of 236****Title:** Conserved Dynamic Mechanism of Allosteric Response to L-arg in Divergent Bacterial Arginine Repressors**Author(s):** Pandey, SK (Pandey, Saurabh Kumar); Melicherick, M (Melicherick, Milan); Reha, D (Reha, David); Ettrich, RH (Ettrich, Rudiger H.); Carey, J (Carey, Jannette)**Source:** MOLECULES **Volume:** 25 **Issue:** 9 **Article Number:** 2247 **DOI:** 10.3390/molecules25092247 **Published:** MAY 2020

**Abstract:** Hexameric arginine repressor, ArgR, is the feedback regulator of bacterial L-arginine regulons, and sensor of L-arg that controls transcription of genes for its synthesis and catabolism. Although ArgR function, as well as its secondary, tertiary, and quaternary structures, is essentially the same in *E. coli* and *B. subtilis*, the two proteins differ significantly in sequence, including residues implicated in the response to L-arg. Molecular dynamics simulations are used here to evaluate the behavior of intact *B. subtilis* ArgR with and without L-arg, and are compared with prior MD results for a domain fragment of *E. coli* ArgR. Relative to its crystal structure, *B. subtilis* ArgR in absence of L-arg undergoes a large-scale rotational shift of its trimeric subassemblies that is very similar to that observed in the *E. coli* protein, but the residues driving rotation have distinct secondary and tertiary structural locations, and a key residue that drives rotation in *E. coli* is missing in *B. subtilis*. The similarity of trimer rotation despite different driving residues suggests that a rotational shift between trimers is integral to ArgR function. This conclusion is supported by phylogenetic analysis of distant ArgR homologs reported here that indicates at least three major groups characterized by distinct sequence motifs but predicted to undergo a common rotational transition. The dynamic consequences of L-arg binding for transcriptional activation of intact ArgR are evaluated here for the first time in two-microsecond simulations of *B. subtilis* ArgR. L-arg binding to intact *B. subtilis* ArgR causes a significant further shift in the angle of rotation between trimers that causes the N-terminal DNA-binding domains lose their interactions with the C-terminal domains, and is likely the first step toward adopting DNA-binding-competent conformations. The results aid interpretation of crystal structures of ArgR and ArgR-DNA complexes.

**Accession Number:** WOS:000535695900243**PubMed ID:** 32397647**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Reha, David		0000-0002-9500-0569

eISSN: 1420-3049

**Record 202 of 236****Title:** Automated construction of bounded-loss imperfect-recall abstractions in extensive-form games**Author(s):** Cermak, J (Cermak, Jiri); Lisy, V (Lisy, Viliam); Bosansky, B (Bosansky, Branislav)**Source:** ARTIFICIAL INTELLIGENCE **Volume:** 282 **Article Number:** 103248 **DOI:** 10.1016/j.artint.2020.103248 **Published:** MAY 2020

**Abstract:** Extensive-form games (EFGs) model finite sequential interactions between players. The amount of memory required to represent these games is the main bottleneck of algorithms for computing optimal strategies and the size of these strategies is often impractical for real-world applications. A common approach to tackle the memory bottleneck is to use information abstraction that removes parts of information available to players thus reducing the number of decision points in the game. However, existing information-abstraction techniques are either specific for a particular domain, they do not provide any quality guarantees, or they are applicable to very small subclasses of EFGs. We present domain-independent abstraction methods for creating imperfect recall abstractions in extensive-form games that allow computing strategies that are (near) optimal in the original game. To this end, we introduce two novel algorithms, FPIRA and CFR+IRA, based on fictitious play and counterfactual regret minimization. These algorithms can start with an arbitrary domain specific, or the coarsest possible, abstraction of the original game. The algorithms iteratively detect the missing information they require for computing a strategy for the abstract game that is (near) optimal in the original game. This information is then included back into the abstract game. Moreover, our algorithms are able to exploit imperfect-recall abstractions that allow players to forget even history of their own actions. However, the algorithms require traversing the complete unabstracted game tree. We experimentally show that our algorithms can closely approximate Nash equilibrium of large games using abstraction with as little as 0.9% of information sets of the original game. Moreover, the results suggest that memory savings increase with the increasing size of the original games. (C) 2020 Elsevier B.V. All rights reserved.

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**Record 203 of 236****Title:** Post-critical behavior of an auto-parametric aero-elastic system with two degrees of freedom**Author(s):** Naprstek, J (Naprstek, J.); Fischer, C (Fischer, C.)**Source:** INTERNATIONAL JOURNAL OF NON-LINEAR MECHANICS **Volume:** 121 **Article Number:** 103441 **DOI:** 10.1016/j.ijnonlinmec.2020.103441 **Published:** MAY 2020

**Abstract:** A generalized two-degree-of-freedom non-linear mathematical system with non-linear gyroscopic and non-conservative terms was used to set up a model for heave and pitch self-excited motion. The stability conditions for a girder with a bluff cross-section in wind flow were identified and presented. The analysis, based on the Routh-Hurwitz conditions and a numerical evaluation of the model, comprises both the self-excited case and an assumption of a harmonic load. The boundaries between different response types that depend on the frequencies of two principal aero-elastic modes are shown. The properties of the response located at these limits and the tendencies of the response in their neighborhood are discussed. The results can be used to explain several experimentally observed effects.

**Accession Number:** WOS:000527346800013**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Naprstek, Jiri F-5871-2013		0000-0002-2323-8439
Fischer, Cyril A-9758-2013		0000-0003-1119-275X

ISSN: 0020-7462

eISSN: 1878-5638

**Record 204 of 236****Title:** Pressure dependence of vibrational optical activity of model biomolecules. A computational study**Author(s):** Plamitzer, L (Plamitzer, Lubos); Bour, P (Bour, Petr)**Source:** CHIRALITY **Volume:** 32 **Issue:** 5 **Pages:** 710-721 **DOI:** 10.1002/chir.23216 **Published:** MAY 2020

**Abstract:** Change of molecular properties with pressure is an attracting means to regulate molecular reactivity or biological activity. However, the effect is usually small and so far explored rather scarcely. To obtain a deeper insight and estimate the sensitivity of vibrational optical activity spectra to pressure-induced conformational changes, we investigate small model molecules. The Ala-Ala dipeptide, isomaltose disaccharide and adenine-uracil dinucleotide were chosen to represent three different biomolecular classes. The pressure effects were modeled by molecular dynamics and density functional theory simulations. The dinucleotide was found to be the most sensitive to the pressure, whereas for the disaccharide the smallest changes are predicted. Pressure-induced relative intensity changes in vibrational circular dichroism and Raman optical activity spectra are predicted to be 2-3-times larger than for non-polarized IR and Raman techniques.

**Accession Number:** WOS:000525865700020**PubMed ID:** 32150771**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Plamitzer, Lubos		0000-0001-8389-9186

ISSN: 0899-0042

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**Record 205 of 236****Title:** Partitioning of polymers between bulk and porous media: Monte Carlo study of the effect of pore size distribution**Author(s):** Wang, X (Wang, Xiu); Prochazka, K (Prochazka, Karel); Limpouchova, Z (Limpouchova, Zuzana)**Source:** JOURNAL OF COLLOID AND INTERFACE SCIENCE **Volume:** 567 **Pages:** 103-112 **DOI:** 10.1016/j.jcis.2020.01.119 **Published:** MAY 1 2020

**Abstract:** In this paper we investigated the partitioning of polymer chains between bulk solvent and porous stationary phase under conditions appropriate for the chromatography under critical conditions (LCCC) close to the critical adsorption point (CAP). We addressed the concentration effect and the thermodynamic effect of pore-size dispersity (PSD) and their impacts on chromatography, i.e., the topics which surprisingly escaped from the interest of scientists in spite that the hydrodynamic effect of PSD has been a subject of numerous studies. The phase equilibria in narrow pores (as compared with the size of polymer coil) with attractive pores are complex and the enthalpy-to-entropy interplay is very intricate. The chains are attracted into pores and the partition coefficients are larger than 1, which corresponds to the interaction chromatography (IC), but they are strongly confined and deformed. The entropy plays important role and the elution volumes of chains differing in molar mass correspond to the size-exclusion chromatography (SEC). The study thus reveals a new chromatography regime which could be easily overlooked without the awareness of its existence. The unexpected findings are important not only for chromatography, but for understanding the phase equilibria of polymers in porous systems in general. (C) 2020 Elsevier Inc. All rights reserved.

**Accession Number:** WOS:000522141900012

**PubMed ID:** 32044539

**Author Identifiers:**

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

ISSN: 0021-9797

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**Record 206 of 236**

**Title:** Predictive compression of molecular dynamics trajectories

**Author(s):** Dvorak, J (Dvorak, Jan); Manak, M (Manak, Martin); Vasa, L (Vasa, Libor)

**Source:** JOURNAL OF MOLECULAR GRAPHICS & MODELLING **Volume:** 96 **Article Number:** 107531 **DOI:** 10.1016/j.jmgm.2020.107531 **Published:** MAY 2020

**Abstract:** Molecular dynamics simulations help to understand the complex behavior of molecules. The output of such a simulation describes the trajectories of individual atoms as snapshots of atom positions in time. Many compression schemes were developed to reduce the amount of data needed for storing long trajectories. This is achieved by limiting the precision of coordinates, encoding differences instead of absolute values, dimensionality reduction by principal component analysis, or by using polynomials approximating vertex trajectories. However, compression schemes using actual bonds between atoms have not been utilized to their full potential. Therefore, we developed a lossy compression method that captures the local, mostly rotational movement of atoms with respect to their bonded neighbors and predicts their positions in each frame. This allows full control over the data distortion. In our experiments, the method achieves data rates which are substantially better than the rates achieved by competing methods at the same error level. (C) 2020 Elsevier Inc. All rights reserved.

**Accession Number:** WOS:000515207000028

**PubMed ID:** 32000011

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Dvorak, Jan	AAR-5455-2020	0000-0003-4569-1151
Manak, Martin		0000-0002-1248-7042

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**Record 207 of 236**

**Title:** Agonist-Specific Conformations of the M-2 Muscarinic Acetylcholine Receptor Assessed by Molecular Dynamics

**Author(s):** Randakova, A (Randakova, Alena); Nelic, D (Nelic, Dominik); Dolezal, V (Dolezal, Vladimir); El-Fakahany, EE (El-Fakahany, Esam E.); Boulos, J (Boulos, John); Jakubik, J (Jakubik, Jan)

**Source:** JOURNAL OF CHEMICAL INFORMATION AND MODELING **Volume:** 60 **Issue:** 4 **Pages:** 2325-2338 **DOI:** 10.1021/acs.jcim.0c00041 **Published:** APR 27 2020

**Abstract:** Binding of muscarinic ligands, both antagonists and agonists, and their effects on the conformation of the M-2 acetylcholine receptor were modeled in silico and compared to experimental data. After docking of antagonists to the M-2 receptor in an inactive conformation (3UON, 5ZK3, 5ZKB, or 5ZKB) and agonists in an active conformation (4MQS), 100 ns of conventional molecular dynamics (MD) followed by 500 ns of accelerated MD was run. Conventional MD revealed ligand-specific interactions with the receptor. Antagonists stabilized the receptor in an inactive conformation during accelerated MD. The receptor in complex with various agonists attained different conformations specific to individual agonists. The magnitude of the TM6 movement correlated with agonist efficacy at the non-preferential G(s) pathway. The shape of the intracellular opening where the receptor interacts with a G-protein was different for the classical agonist carbachol, super-agonist iperoxo, and G(i/o)-biased partial agonists JR-6 and JR-7, being compatible with experimentally observed agonist bias at the G-protein level. Moreover, a wash-resistant binding of the unique agonist xanomeline associated with interactions with membrane lipids was formed during accelerated MD. Thus, accelerated MD is suitable for modeling of ligand-specific receptor binding and receptor conformations that is essential for the design of experiments aimed at identification of the secondary binding sites and understanding molecular mechanisms underlying receptor activation.

**Accession Number:** WOS:000529208800038

**PubMed ID:** 32130001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Jakubik, Jan	B-7461-2012	0000-0002-1737-1487
Dolezal, Vladimir	A-8732-2008	0000-0003-3412-256X
Randakova, Alena		0000-0002-8403-6494

ISSN: 1549-9596

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**Record 208 of 236**

**Title:** Ergodicity Breaking in Thermal Biological Electron Transfer? Cytochrome C Revisited II

**Author(s):** Futera, Z (Futera, Zdenek); Jiang, XY (Jiang, Xiuyun); Blumberger, J (Blumberger, Jochen)

**Source:** JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 124 **Issue:** 16 **Pages:** 3336-3342 **DOI:** 10.1021/acs.jpcc.0c01414 **Published:** APR 23 2020

**Abstract:** It was recently suggested that cytochrome c operates in an ergodicity-breaking regime characterized by unusually large energy gap thermal fluctuations and associated reorganization free energies for heme oxidation of up to 3.0 eV. The large fluctuations were reported to lower activation free energy for oxidation of the heme cofactor by almost a factor of 2 compared to the case where ergodicity is maintained. Our group has recently investigated this claim computationally at several levels of theory and found no evidence for such large energy gap fluctuations. Here we address the points of our earlier work that have raised criticism and we also extend our previous investigation by considering a simple linear polarizability model for cytochrome c oxidation. We find very consistent results among all our computational approaches, ranging from classical molecular dynamics, to the linear polarizability model to QM(PMM)/MM to full QM(DFT)/MM electrostatic embedding. None of them support the notion of very large energy gap fluctuations or ergodicity breaking. The deviation between our simulations and the ones reported in [J. Phys. Chem. B 2017, 121, 4958] is traced back to rather large electric fields at the Fe site of the heme c cofactor in that study, not seen in our simulations, neither with the AMBER nor with the CHARMM force field. While ergodicity breaking effects may well occur in other biological ET, our numerical evidence suggests that this is not the case for cytochrome c.

**Accession Number:** WOS:000529216600010

**PubMed ID:** 32223243

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Futera, Zdenek	F-8771-2015	0000-0003-0471-8194

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**Record 209 of 236**

**Title:** Stellar wind models of central stars of planetary nebulae

**Author(s):** Krticka, J (Krticka, J.); Kubat, J (Kubat, J.); Krtickova, I (Krtickova, I)

**Source:** ASTRONOMY & ASTROPHYSICS **Volume:** 635 **DOI:** 10.1051/0004-6361/201937150 **Published:** APR 2 2020



**Abstract:** Context. Fast line-driven stellar winds play an important role in the evolution of planetary nebulae, even though they are relatively weak. Aims. We provide global (unified) hot star wind models of central stars of planetary nebulae. The models predict wind structure including the mass-loss rates, terminal velocities, and emergent fluxes from basic stellar parameters. Methods. We applied our wind code for parameters corresponding to evolutionary stages between the asymptotic giant branch and white dwarf phases for a star with a final mass of 0.569  $M_{\odot}$ . We study the influence of metallicity and wind inhomogeneities (clumping) on the wind properties. Results. Line-driven winds appear very early after the star leaves the asymptotic giant branch (at the latest for T-eff approximate to 10 kK) and fade away at the white dwarf cooling track (below T-eff = 105 kK). Their mass-loss rate mostly scales with the stellar luminosity and, consequently, the mass-loss rate only varies slightly during the transition from the red to the blue part of the Hertzsprung-Russell diagram. There are the following two exceptions to the monotonic behavior: a bistability jump at around 20 kK, where the mass-loss rate decreases by a factor of a few (during evolution) due to a change in iron ionization, and an additional maximum at about T-eff = 40-50 kK. On the other hand, the terminal velocity increases from about a few hundreds of km s<sup>-1</sup> to a few thousands of km s<sup>-1</sup> during the transition as a result of stellar radius decrease. The wind terminal velocity also significantly increases at the bistability jump. Derived wind parameters reasonably agree with observations. The effect of clumping is stronger at the hot side of the bistability jump than at the cool side. Conclusions. Derived fits to wind parameters can be used in evolutionary models and in studies of planetary nebula formation. A predicted bistability jump in mass-loss rates can cause the appearance of an additional shell of planetary nebula.

**Accession Number:** WOS:000526658700001

**Author Identifiers:**

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

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#### Record 210 of 236

**Title:** Synthesis and computational mechanistic studies of copper selective molecular receptor

**Author(s):** Mohan, B (Mohan, Brij); Modi, K (Modi, Krupal); Patel, C (Patel, Chirag); Kumar, S (Kumar, Sandeep); Sharma, HK (Sharma, Harish Kumar)

**Source:** VIETNAM JOURNAL OF CHEMISTRY **Volume:** 58 **Issue:** 2 **Pages:** 221-230 **DOI:** 10.1002/vjch.201900161 **Published:** APR 2020

**Abstract:** Although numerous molecular receptors for Cu<sup>2+</sup> have been reported, it is not obvious to find a simple molecule as a selective receptor for Cu<sup>2+</sup>. Here we create a molecular receptor 4MHEB for Cu<sup>2+</sup> metal ions. Observation of a new absorption band near 282 nm in UV-visible spectra and enhancement in fluorescence intensity in emission spectra justify the binding 4MHEB:Cu<sup>2+</sup> binding. Inspection in shifting of IR bands, different thermal behavior and oxidation and reduction peaks of complex shows binding of 4MHEB:Cu<sup>2+</sup>. HRMS m/z 322.0328, Benesi-Hildebrand method and Job's Plot results 1:1 (4MHEB:Cu<sup>2+</sup>) binding stoichiometry with the binding affinity K = 1.751x10<sup>5</sup> M<sup>-1</sup>. The docked pose of 4MHEB with Cu<sup>2+</sup> ion, Key transitions, % Contribution was calculated by computational studies.

**Accession Number:** WOS:000588009800014

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#### Record 211 of 236

**Title:** Catalase and Ascorbate Peroxidase in Euglenozoan Protists

**Author(s):** Skodova-Sverakova, I (Skodova-Sverakova, Ingrid); Zahonova, K (Zahonova, Kristina); Buckkova, B (Buckkova, Barbora); Fussy, Z (Fussy, Zoltan); Yurchenko, V (Yurchenko, Vyacheslav); Lukes, J (Lukes, Julius)

**Source:** PATHOGENS **Volume:** 9 **Issue:** 4 **Article Number:** 317 **DOI:** 10.3390/pathogens9040317 **Published:** APR 2020

**Abstract:** In this work, we studied the biochemical properties and evolutionary histories of catalase (CAT) and ascorbate peroxidase (APX), two central enzymes of reactive oxygen species detoxification, across the highly diverse clade Euglenozoa. This clade encompasses free-living phototrophic and heterotrophic flagellates, as well as obligate parasites of insects, vertebrates, and plants. We present evidence of several independent acquisitions of CAT by horizontal gene transfers and evolutionary novelties associated with the APX presence. We posit that Euglenozoa recruit these detoxifying enzymes for specific molecular tasks, such as photosynthesis in euglenids and membrane-bound peroxidase activity in kinetoplastids and some diplomonids.

**Accession Number:** WOS:000534051600058

**PubMed ID:** 32344595

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lukes, Julius	H-6760-2012	0000-0002-0578-6618
Zahonova, Kristina	AAT-9188-2020	0000-0002-5766-0267
Yurchenko, Vyacheslav	E-4532-2013	0000-0003-4765-3263
Fussy, Zoltan	A-6025-2013	0000-0002-0820-6359
Sverakova, Ingrid		0000-0002-4004-3377

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#### Record 212 of 236

**Title:** Distorted surfaces of magnetic helium-peculiar stars: an application to a Cen

**Author(s):** Krticka, J (Krticka, J.); Mikulasek, Z (Mikulasek, Z.); Prvak, M (Prvak, M.); Niemczura, E (Niemczura, E.); Leone, F (Leone, F.); Wade, G (Wade, G.)

**Source:** MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY **Volume:** 493 **Issue:** 2 **Pages:** 2140-2148 **DOI:** 10.1093/mnras/staa378 **Published:** APR 2020

**Abstract:** Helium-peculiar magnetic chemically peculiar stars show variations of helium abundance across their surfaces. As a result of associated atmospheric scale height variations, the stellar surface becomes distorted, with helium-rich regions bent inwards. Effectively, on top of flux variations due to opacity effects, the depressed helium-rich surface regions become less bright in the optical regions and brighter in the ultraviolet. We study the observational effects of the aspherical surface on the light curves of a Cen. We simulate the light curves of this star adopting surface distributions of He, N, O, Si, and Fe derived from Doppler mapping and introducing the effect of distortion proportional to helium abundance. We show that while most of the optical and UV variations of this star result from flux redistribution due to the non-uniform surface distributions of helium and iron, the reduction of light variations due to the helium-related surface distortion leads to a better agreement between simulated optical light curves and the light curves observed with the BRITE satellites.

**Accession Number:** WOS:000525996700042

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Leone, Francesco	AAO-7001-2020	0000-0001-7626-3788
Niemczura, Ewa		0000-0001-7290-5800

ISSN: 0035-8711

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#### Record 213 of 236

**Title:** Re-examining the interpretation of CO adsorbed on Lewis acid sites of alkali metal-exchanged MOR zeolite

**Author(s):** Bulanek, R (Bulanek, Roman); Koudelkova, E (Koudelkova, Eva); Trachta, M (Trachta, Michal); Bludsky, O (Bludsky, Ota); Rubes, M (Rubes, Miroslav)

**Source:** MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 296 **Article Number:** 110007 **DOI:** 10.1016/j.micromeso.2020.110007 **Published:** APR 2020

**Abstract:** The interaction of CO with alkali metal-exchanged mordenite has been investigated by means of IR spectroscopy and calorimetry along with theoretical calculations based on DFT corrected to coupled-cluster accuracy (DFT/CC). It has been convincingly shown that Li<sup>+</sup> is at least partially exchanged into the constricted part of the MOR structure as manifested by the low-frequency band at 2181 cm<sup>-1</sup> and the isosteric heat of 44 kJ/mol. In the case of Na-MOR samples, significant changes have been observed in the stabilities of high- (2177 cm<sup>-1</sup>) and low-frequency (2165 cm<sup>-1</sup>) bands upon CO desorption, with the change of the Si/Al ratio from 40 to 9. Based on the kinetic measurements, it can be concluded that a crucial role in the MOR material is played by diffusion limitations, which are significantly influenced by the Si/Al ratio and the size of the cations. Similar effects also result in the increased stability of the 2138 cm<sup>-1</sup> band of Na/K-MOR samples with higher Al content, where the "gate" effect is observed upon N<sub>2</sub> adsorption. The dual cationic sites are directly observed only for the K-MOR sample via the weak band around 2150 cm<sup>-1</sup>. The formation of dual cationic sites cannot be completely ruled out in the case of Na-MOR, but their presence is most likely hidden in the low-frequency band.

**Accession Number:** WOS:000518494800028

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Rubes, Miroslav	G-7997-2014	0000-0002-9213-0915

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**Record 214 of 236****Title:** The Beta Subunit of Nascent Polypeptide Associated Complex Plays A Role in Flowers and Siliques Development of *Arabidopsis thaliana***Author(s):** Fila, J (Fila, Jan); Klodova, B (Klodova, Bozena); Potesil, D (Potesil, David); Juricek, M (Juricek, Miloslav); Sestak, P (Sestak, Petr); Zdrahal, Z (Zdrahal, Zbynek); Honys, D (Honys, David)**Source:** INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES **Volume:** 21 **Issue:** 6 **Article Number:** 2065 **DOI:** 10.3390/ijms21062065 **Published:** MAR 2020

**Abstract:** The nascent polypeptide-associated (NAC) complex was described in yeast as a heterodimer composed of two subunits, alpha and beta, and was shown to bind to the nascent polypeptides newly emerging from the ribosomes. NAC function was widely described in yeast and several information are also available about its role in plants. The knock down of individual NAC subunit(s) led usually to a higher sensitivity to stress. In *Arabidopsis thaliana* genome, there are five genes encoding NAC alpha subunit, and two genes encoding NAC beta. Double homozygous mutant in both genes coding for NAC beta was acquired, which showed a delayed development compared to the wild type, had abnormal number of flower organs, shorter siliques and greatly reduced seed set. Both NAC beta genes were characterized in more detail-the phenotype of the double homozygous mutant was complemented by a functional NAC beta copy. Then, both NAC beta genes were localized to nuclei and cytoplasm and their promoters were active in many organs (leaves, cauline leaves, flowers, pollen grains, and siliques together with seeds). Since flowers were the most affected organs by nac beta mutation, the flower buds' transcriptome was identified by RNA sequencing, and their proteome by gel-free approach. The differential expression analyses of transcriptomic and proteomic datasets suggest the involvement of NAC beta subunits in stress responses, male gametophyte development, and photosynthesis.

**Accession Number:** WOS:000529890200161**PubMed ID:** 32192231**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Fila, Jan	G-2102-2011	0000-0002-5774-0136
Potesil, David	D-9696-2012	0000-0003-0390-0904
Zdrahal, Zbynek		0000-0003-3044-5548

eISSN: 1422-0067

**Record 215 of 236****Title:** Structural Basis of Ca<sup>2+</sup>-Dependent Self-Processing Activity of Repeat-in-Toxin Proteins**Author(s):** Kuban, V (Kuban, Vojtech); Macek, P (Macek, Pavel); Hritz, J (Hritz, Jozef); Nechvatalova, K (Nechvatalova, Katerina); Nedbalcova, K (Nedbalcova, Katerina); Faldyna, M (Faldyna, Martin); Sebo, P (Sebo, Peter); Zidek, L (Zidek, Lukas); Bumba, L (Bumba, Ladislav)**Source:** MBIO **Volume:** 11 **Issue:** 2 **Article Number:** e00226-20 **DOI:** 10.1128/mBio.00226-20 **Published:** MAR-APR 2020

**Abstract:** The posttranslational Ca<sup>2+</sup>-dependent "clip-and-link" activity of large repeat-in-toxin (RTX) proteins starts by Ca<sup>2+</sup>-dependent structural rearrangement of a highly conserved self-processing module (SPM). Subsequently, an internal aspartate-proline (Asp-Pro) peptide bond at the N-terminal end of SPM breaks, and the liberated C-terminal aspartyl residue can react with a free epsilon-amino group of an adjacent lysine residue to form a new isopeptide bond. Here, we report a solution structure of the calcium-loaded SPM (Ca-SPM) derived from the FrpC protein of *Neisseria meningitidis*. The Ca-SPM structure defines a unique protein architecture and provides structural insight into the autocatalytic cleavage of the Asp-Pro peptide bond through a "twisted-amide" activation. Furthermore, in-frame deletion of the SPM domain from the ApxIVA protein of *Actinobacillus pleuropneumoniae* attenuated the virulence of this porcine pathogen in a pig respiratory challenge model. We hypothesize that the Ca<sup>2+</sup>-dependent clip-and-link activity represents an unconventional strategy for Gram-negative pathogens to adhere to the host target cell surface.

**IMPORTANCE** The Ca<sup>2+</sup>-dependent clip-and-link activity of large repeat-in-toxin (RTX) proteins is an exceptional posttranslational process in which an internal domain called a self-processing module (SPM) mediates Ca<sup>2+</sup>-dependent processing of a highly specific aspartate-proline (Asp-Pro) peptide bond and covalent linkage of the released aspartyl to an adjacent lysine residue through an isopeptide bond. Here, we report the solution structures of the Ca<sup>2+</sup>-loaded SPM (Ca-SPM) defining the mechanism of the autocatalytic cleavage of the Asp414-Pro415 peptide bond of the *Neisseria meningitidis* FrpC exoprotein. Moreover, deletion of the SPM domain in the ApxIVA protein, the FrpC homolog of *Actinobacillus pleuropneumoniae*, resulted in attenuation of virulence of the bacterium in a pig infection model, indicating that the Ca<sup>2+</sup>-dependent clip-and-link activity plays a role in the virulence of Gram-negative pathogens.

**Accession Number:** WOS:000531071300056**PubMed ID:** 32184239**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
SEBO, Peter	N-2043-2019	0000-0002-9755-7715
SEBO, Peter	F-7423-2011	0000-0002-9755-7715
Hritz, Jozef	J-6887-2015	0000-0002-4512-9241
Zidek, Lukas	D-7112-2012	0000-0002-8013-0336
Bumba, Ladislav	ABC-9943-2020	0000-0001-6659-5447

ISSN: 2150-7511

**Record 216 of 236****Title:** Classification with costly features as a sequential decision-making problem**Author(s):** Janisch, J (Janisch, Jaromir); Pevny, T (Pevny, Tomas); Lisy, V (Lisy, Viliam)**Source:** MACHINE LEARNING **Volume:** 109 **Issue:** 8 **Pages:** 1587-1615 **DOI:** 10.1007/s10994-020-05874-8 **Early Access Date:** FEB 2020 **Published:** AUG 2020

**Abstract:** This work focuses on a specific classification problem, where the information about a sample is not readily available, but has to be acquired for a cost, and there is a per-sample budget. Inspired by real-world use-cases, we analyze average and hard variations of a directly specified budget. We postulate the problem in its explicit formulation and then convert it into an equivalent MDP, that can be solved with deep reinforcement learning. Also, we evaluate a real-world inspired setting with sparse training datasets with missing features. The presented method performs robustly well in all settings across several distinct datasets, outperforming other prior-art algorithms. The method is flexible, as showcased with all mentioned modifications and can be improved with any domain independent advancement in RL.

**Accession Number:** WOS:000517008900001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Janisch, Jaromir		0000-0002-4165-6503

ISSN: 0885-6125

eISSN: 1573-0565

**Record 217 of 236****Title:** Proper treatment of the Pauli principle in mirror nuclei within the microscopic particle(hole)-phonon scheme**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:** 101 **Issue:** 2 **Article Number:** 024308 **DOI:** 10.1103/PhysRevC.101.024308 **Published:** FEB 19 2020

**Abstract:** It is shown that the Cholesky decomposition method, implemented in mirror nuclei to extract an orthonormal basis from a redundant set of states composed of a valence particle (hole) coupled to Tamm-Dancoff approximation (TDA) phonons, yields a few levels which violate the mirror symmetry, at variance with the shell model. A more appropriate implementation of the method is suggested which eliminates this inconsistency.

**Accession Number:** WOS:000514686000003**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290

De Gregorio, Giovanni 0000-0003-0253-915X

ISSN: 2469-9985

eISSN: 2469-9993

**Record 218 of 236****Title:** Controlling Single Molecule Conductance by a Locally Induced Chemical Reaction on Individual Thiophene Units**Author(s):** Michnowicz, T (Michnowicz, Tomasz); Borca, B (Borca, Bogdana); Petuya, R (Petuya, Remi); Schendel, V (Schendel, Verena); Pristl, M (Pristl, Marcel); Pentegov, I (Pentegov, Ivan); Kraft, U (Kraft, Ulrike); Klauk, H (Klauk, Hagen); Wahl, P (Wahl, Peter); Mutombo, P (Mutombo, Pingo); Jelinek, P (Jelinek, Pavel); Arnau, A (Arnau, Andres); Schlickum, U (Schlickum, Uta); Kern, K (Kern, Klaus)**Source:** ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 59 **Issue:** 15 **Pages:** 6207-6212 **DOI:** 10.1002/anie.201915200 **Early Access Date:** FEB 2020 **Published:** APR 6 2020**Abstract:** Among the prerequisites for the progress of single-molecule-based electronic devices are a better understanding of the electronic properties at the individual molecular level and the development of methods to tune the charge transport through molecular junctions. Scanning tunneling microscopy (STM) is an ideal tool not only for the characterization, but also for the manipulation of single atoms and molecules on surfaces. The conductance through a single molecule can be measured by contacting the molecule with atomic precision and forming a molecular bridge between the metallic STM tip electrode and the metallic surface electrode. The parameters affecting the conductance are mainly related to their electronic structure and to the coupling to the metallic electrodes. Here, the experimental and theoretical analyses are focused on single tetraceno thiophene molecules and demonstrate that an in situ-induced direct desulfurization reaction of the thiophene moiety strongly improves the molecular anchoring by forming covalent bonds between molecular carbon and copper surface atoms. This bond formation leads to an increase of the conductance by about 50 % compared to the initial state.**Accession Number:** WOS:000513999600001**PubMed ID:** 31965698**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Wahl, Peter	F-9337-2014	0000-0002-8635-1519
Jelinek, Pavel	ABE-8589-2020	0000-0002-5645-8542
Kraft, Ulrike		0000-0002-2104-9706
Mutombo, Pingo	G-5266-2014	0000-0002-8175-7587
Petuya, Remi	C-1147-2015	0000-0002-3118-6966
ARNAU PINO, ANDRES	H-7901-2012	0000-0001-5281-3212
Borca, Bogdana		0000-0001-5485-4536

ISSN: 1433-7851

eISSN: 1521-3773

**Record 219 of 236****Title:** Modelling of inhomogeneous mixing of plasma species in argon-steam arc discharge for broad range of operating conditions**Author(s):** Jenista, J (Jenista, Jiri); Takana, H (Takana, Hidemasa); Nishiyama, H (Nishiyama, Hideya); Bartlova, M (Bartlova, Milada); Aubrecht, V (Aubrecht, Vladimir); Murphy, AB (Murphy, Anthony B.)**Source:** EUROPEAN PHYSICAL JOURNAL D **Volume:** 74 **Issue:** 2 **Article Number:** 22 **DOI:** 10.1140/epjd/e2019-100254-3 **Published:** FEB 4 2020**Abstract:** Numerical simulation of mixing of argon- and water-plasma species in argon-steam arc discharge has been investigated in thermal plasma generator with the combined stabilization of arc by axial gas flow (argon) and water vortex. Mixing process is described by the combined diffusion coefficients method in which the coefficients describe the diffusion of argon "gas", with respect to steam "gas". Calculations for currents 150-600 A with 15-40 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. However, calculations for currents higher than 400 A were not straightforward and a phenomenon of premixing of argon and steam species in the upstream discharge region was predicted from modelling to obtain reasonable agreement with experimental data. Premixed argon-steam plasma has a global impact on the plasma jet parameters near the exit nozzle as well as on the overall arc performance. The results of thermo-fluid fields, species mole fractions and radiation losses from the discharge are presented and discussed. Our former calculations based on the homogeneous mixing assumption differ from the present model in temperature, enthalpy, radiation losses, and flow field. Comparison with available experiments exhibits very good qualitative and quantitative agreements for the radial temperature profiles and satisfactory agreement for the velocity profiles 2 mm downstream of the exit nozzle.**Accession Number:** WOS:000513232300003**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Murphy, Anthony B	A-7796-2008	0000-0002-2820-2304
Jenista, Jiri		0000-0002-6544-9234

ISSN: 1434-6060

eISSN: 1434-6079

**Record 220 of 236****Title:** Laser wakefield accelerator driven by the super-Gaussian laser beam in the focus**Author(s):** Maslarova, D (Maslarova, Dominika); Krus, M (Krus, Miroslav); Horny, V (Horny, Vojtech); Psikal, J (Psikal, Jan)**Source:** PLASMA PHYSICS AND CONTROLLED FUSION **Volume:** 62 **Issue:** 2 **Article Number:** 024005 **DOI:** 10.1088/1361-6587/ab57ee **Published:** FEB 2020**Abstract:** The injection process is one of the most crucial attributes that determine the final properties of the electron bunch in laser wakefield accelerators. Here, a new injection method is proposed and studied via particle-in-cell simulations for the typical parameters of the bubble regime. The injection is triggered by the laser beam that reaches the super-Gaussian profile in the focus. Such a beam undergoes rapid variations in its intensity distribution during the diffraction process. If this diffraction occurs in underdense plasma, consequent changes in the bubble structure activate a localized transverse injection process. The generated electron bunch is characterized by the short duration (similar to 2 fs) and low transverse emittance ( $\leq 1$  mm mrad) while maintaining relatively high charge (similar to 0.2 nC).**Accession Number:** WOS:000537378100001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Horny, Vojtech	Q-4792-2018	0000-0002-4510-3770
Psikal, Jan	G-8403-2014	0000-0003-4586-1149
Maslarova, Dominika		0000-0002-2756-3722

ISSN: 0741-3335

eISSN: 1361-6587

**Record 221 of 236****Title:** Stability of small vacancy clusters in tungsten by molecular dynamics**Author(s):** Fikar, J (Fikar, Jan); Schaublin, R (Schaublin, Robin)**Source:** NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS **Volume:** 464 **Pages:** 56-59 **DOI:** 10.1016/j.nimb.2019.11.044 **Published:** FEB 1 2020**Abstract:** The vacancies produced in collision cascades of irradiated metals form voids and vacancy clusters. The stability of vacancy clusters and voids is usually studied by kinetic Monte-Carlo methods. We investigated the stability of these vacancy defects at high temperatures using molecular dynamics and recent embedded-atom method potential. We confirm that the vacancy cluster dissociation is thermally activated. We have obtained dissociation energies and characteristic temperatures, both increasing with the number of vacancies and tending to saturate at 3.5 eV and 1200 K, respectively, for large vacancy clusters. Our results qualitatively agree with Monte-Carlo results, but predict somewhat smaller values for both the dissociation energy and characteristic temperature.**Accession Number:** WOS:000510313800011**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Fikar, Jan	G-4365-2014	0000-0003-1499-3958
Schaublin, Robin	O-1426-2016	0000-0002-8379-9705



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eISSN: 1872-9584

#### Record 222 of 236

**Title:** Molecular dynamics of aqueous salt solutions in clay nanopores under the thermodynamic conditions of hydraulic fracturing: Interplay between solution structure and molecular diffusion

**Author(s):** Plankova, B (Plankova, Barbora); Lisal, M (Lisal, Martin)

**Source:** FLUID PHASE EQUILIBRIA **Volume:** 505 **Article Number:** 112355 **DOI:** 10.1016/j.fluid.2019.112355 **Published:** FEB 1 2020

**Abstract:** Shale gas has become an important unconventional energy resource and is extracted by hydraulic fracturing of shale rocks. In shale rocks, kerogen and clays are present, the former providing storage for hydrocarbons, the latter preventing hydrocarbon transport. Clays are hydrophilic and have a layered structure. They can adsorb aqueous salt solutions in the interlayer space, and the interlayer ions contribute to a very high salinity of the flow-back water. We used montmorillonite (MMT) as a proxy of clays and study the interplay between the interlayer structure and the molecular diffusion of the aqueous salt solutions confined in the clay nanopores. We considered water with monovalent Na and divalent Ca ions in the MMT slit pores under a typical shale gas reservoir condition of a temperature of 365 K and a pressure of 275 bar. The confined systems were electrostatically balanced by Cl ions. We varied the amount of water to cover one-, two-, three-, and four-layer hydrate states. We quantified the solution structure in terms of the interlayer atomic density profiles, complemented by the charge density and water orientation profiles. We further evaluated the in-plane self-diffusivity of water and ions to provide insight into the diffusion behaviour of the concentrated water-NaCl and water-CaCl<sub>2</sub> solutions in the interlayer galleries of the Na- and Ca-MMT pores. We found that the interlayer water structure displays an attraction of water hydrogens to the clay surfaces as a result of the strong H-bond interactions of water molecules with the surface oxygens and formation of a diffusive layer inside wide clay pores. The presence of divalent Ca ions has more pronounced effects on the interlayer water structures than the monovalent Na ions. Divalent Ca ions exhibit a preference for inner-sphere complexes over outer-sphere complexes due to the strong adsorption on the clay surfaces while Na ions show the opposite trend. The diffusion of water and ions in the clay pores is reduced in comparison with the diffusion in the bulk, especially for the one-layer hydrate states. The presence of the salts in the clay pores further decreases the water diffusion, with a stronger decrease for the divalent CaCl<sub>2</sub> than the monovalent NaCl. The diffusion of small Na<sup>+</sup> and Ca<sup>2+</sup> is lower than large Cl<sup>-</sup> due to the low mobility of the adsorbed cations and the distribution of Cl ions inside the pores where they can diffuse faster. (C) 2019 Elsevier B.V. All rights reserved.

**Accession Number:** WOS:000501403500006

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Lisal, Martin ML A-8176-2011		0000-0001-8005-7143

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eISSN: 1879-0224

#### Record 223 of 236

**Title:** Diastereoselective Cyclopropanation through Michael Addition-Initiated Ring Closure between alpha,alpha-Dibromoketones and alpha,beta-Unsaturated Fischer Carbene Complexes

**Author(s):** Tobrman, T (Tobrman, Tomas); Krupicka, M (Krupicka, Martin); Polak, P (Polak, Peter); Dvorakova, H (Dvorakova, Hana); Cubinak, M (Cubinak, Marek); Babor, M (Babor, Martin); Dvorak, D (Dvorak, Dalimil)

**Source:** EUROPEAN JOURNAL OF ORGANIC CHEMISTRY **Volume:** 2020 **Issue:** 4 **Pages:** 429-436 **DOI:** 10.1002/ejoc.201901503 **Early Access Date:** JAN 2020 **Published:** JAN 31 2020

**Abstract:** The diastereoselective synthesis of tetrasubstituted cyclopropanes is described. The two-step procedure is based on the 3-exo-tet Michael addition-initiated ring closure. In the first step, the enolates derived from alpha,alpha-dibromoketones react with the alpha,beta-unsaturated Fischer alkoxy carbene complexes to obtain tetrasubstituted cyclopropanes, which are then treated with ceric-ammonium nitrate to yield the final products. The methodology tolerates diverse functional groups, and high diastereoselectivity (dr >= 98:2) is observed in all cases.

**Accession Number:** WOS:000507322200001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Babor, Martin	ABC-5252-2020	0000-0002-0268-4640
Krupicka, Martin A-1810-2009		0000-0002-9132-5825
tobrman, tomas		0000-0003-3473-9199

ISSN: 1434-193X

eISSN: 1099-0690

#### Record 224 of 236

**Title:** Near-Wall Flow in the Blade Cascades Representing Last Rotor Root Sections of Large Output Steam Turbines

**Author(s):** Simurda, D (Simurda, David); Furst, J (Furst, Jiri); Hala, J (Hala, Jindrich); Luxa, M (Luxa, Martin); Bobcik, M (Bobcik, Marek); Novak, O (Novak, Ondrej); Synac, J (Synac, Jaroslav)

**Source:** JOURNAL OF THERMAL SCIENCE **DOI:** 10.1007/s11630-020-1246-x **Early Access Date:** JAN 2020

**Abstract:** This paper investigates the flow past two variants of root section profile cascades for a last stage rotor considering three-dimensional flow structures in the near-wall region. Analyses were drawn based on RANS numerical simulations of both variants and on the experimental data obtained by the 3D traversing in the exit flow field of one of the variants. Extent of 3D structures at two different regimes and its influence on aerodynamic characteristics of the blade cascades was assessed. The distributions of Mach number along the profiles were compared with 2D optical measurements and its distortion due to the presence of the sidewall was explored. The interaction between main vortical structures was described and its influence on the loading of the blades, mechanical energy losses and exit flow angle was discussed. The results showed that for a front loaded blade the vortical structures appeared earlier and at a larger extent than for an aft loaded variant. However, due to different Mach number distribution, contribution of end wall flow to the energy losses was lower in the case of the aft loaded variant. The influence of the near wall flow on the loading was found to be rather weak while the deviation of the exit flow angle appeared to be comparable for both of the variants.

**Accession Number:** WOS:000574097200001

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Furst, Jiri	A-8202-2011	0000-0003-3454-8974
Simurda, David H-1340-2014		

ISSN: 1003-2169

eISSN: 1993-033X

#### Record 225 of 236

**Title:** Rotameric Isomers of La-2@C-80& Dodecafluoro-Subphthalocyanine Conjugate: Computational Characterization

**Author(s):** Slanina, Z (Slanina, Zdenek); Uhlík, F (Uhlík, Filip); Feng, L (Feng, Lai); Akasaka, T (Akasaka, Takeshi); Lu, X (Lu, Xing); Adamowicz, L (Adamowicz, Ludwik)

**Source:** ECS JOURNAL OF SOLID STATE SCIENCE AND TECHNOLOGY **Volume:** 9 **Issue:** 6 **Article Number:** 061014 **DOI:** 10.1149/2162-8777/aba0cf **Published:** JAN 8 2020

**Abstract:** Stability and spectra of rotamers of a previously via Prato reaction prepared conjugate of dimetallofullerene La-2@C(80) and dodecafluoro-subphthalocyanine with summary formula C113H10BF12La2N7O and bridging over the cage C-C bond between five- and six-membered rings are calculated. The inter-rotameric energetics is evaluated at the M06-2X/6-311G\* similar to SDD level while the entropy term with the M06-2X/3-21G similar to SDD approach. The rotamer most-populated at room and higher temperatures has a structure in which both the nitrogen atom of the pyrrolidine ring and the dodecafluoro-subphthalocyanine moiety are inclined toward the five-membered ring belonging to the bridged-over C-C bond. The vibrational and electronic spectra are simulated and the latter spectrum agrees with the observed features. The calculated nanocarbon system is about the largest of its type computationally treated so far.

**Accession Number:** WOS:000554506800001

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#### Record 226 of 236

**Title:** The impact of tunnel mutations on enzymatic catalysis depends on the tunnel-substrate complementarity and the rate-limiting step

**Author(s):** Kokkonen, P (Kokkonen, Piia); Slanska, M (Slanska, Michaela); Dockalova, V (Dockalova, Veronika); Pinto, GP (Pinto, Gaspar P.); Sanchez-Carnerero, EM (Sanchez-Carnerero, Esther M.); Damborsky, J (Damborsky, Jiri); Klan, P (Klan, Petr); Prokop, Z (Prokop, Zbynek); Bednar, D (Bednar, David)

**Source:** COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL **Volume:** 18 **Pages:** 805-813 **DOI:** 10.1016/j.csbj.2020.03.017 **Published:** 2020

**Abstract:** Transport of ligands between bulk solvent and the buried active sites is a critical event in the catalytic cycle of many enzymes. The rational design of transport pathways is far from trivial due to the lack of knowledge about the effect of mutations on ligand transport. The main and an auxiliary tunnel of haloalkane dehalogenase LinB have been previously engineered for improved dehalogenation of 1,2-dibromoethane (DBE). The first chemical step of DBE conversion was enhanced by L177W mutation in the main tunnel, but the rate-limiting product release was slowed down because the mutation blocked the main access tunnel and hindered protein dynamics. Three additional mutations W140A + F143L + I211L opened-up the auxiliary tunnel and enhanced the product release, making this four-point variant the most efficient catalyst with DBE. Here we study the impact of these mutations on the catalysis of bulky aromatic substrates, 4-(bromomethyl)-6,7-dimethoxycoumarin (COU) and 8-chloromethyl-4,4'-difluoro-3,5-dimethyl-4-bora-3a,4a-diaza-s-indacene (BDP). The rate-limiting step of DBE conversion is the product release, whereas the catalysis of COU and BDP is limited by the chemical step. The catalysis of COU is mainly impaired by the mutation L177W, whereas the conversion of BDP is affected primarily by the mutations W140A + F143L + I211L. The combined computational and kinetic analyses explain the differences in activities between the enzyme-substrate pairs. The effect of tunnel mutations on catalysis depends on the rate-limiting step, the complementarity of the tunnels with the substrates and is clearly specific for each enzyme-substrate pair. (C) 2020 The Authors. Published by Elsevier B.V. on behalf of Research Network of Computational and Structural Biotechnology.

**Accession Number:** WOS:000607729500006

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**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Klan, Petr	H-1189-2012	0000-0001-6287-2742
Bartos, Piia		0000-0001-6002-1856
Dockalova, Veronika		0000-0002-6606-2058

**ISSN:** 2001-0370

**Record 227 of 236**

**Title:** Structures of hyperstable ancestral haloalkane dehalogenases show restricted conformational dynamics

**Author(s):** Babkova, P (Babkova, Petra); Dunajova, Z (Dunajova, Zuzana); Chaloupkova, R (Chaloupkova, Radka); Damborsky, J (Damborsky, Jiri); Bednar, D (Bednar, David); Marek, M (Marek, Martin)

**Source:** COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL **Volume:** 18 **Pages:** 1497-1508 **DOI:** 10.1016/j.csbj.2020.06.021 **Published:** 2020

**Abstract:** Ancestral sequence reconstruction is a powerful method for inferring ancestors of modern enzymes and for studying structure-function relationships of enzymes. We have previously applied this approach to haloalkane dehalogenases (HLDs) from the subfamily HLD-II and obtained thermodynamically highly stabilized enzymes (Delta T-m up to 24 degrees C), showing improved catalytic properties. Here we combined crystallographic structural analysis and computational molecular dynamics simulations to gain insight into the mechanisms by which ancestral HLDs became more robust enzymes with novel catalytic properties. Reconstructed ancestors exhibited similar structure topology as their descendants with the exception of a few loop deviations. Strikingly, molecular dynamics simulations revealed restricted conformational dynamics of ancestral enzymes, which prefer a single state, in contrast to modern enzymes adopting two different conformational states. The restricted dynamics can potentially be linked to their exceptional stabilization. The study provides molecular insights into protein stabilization due to ancestral sequence reconstruction, which is becoming a widely used approach for obtaining robust protein catalysts. (C) 2020 The Author(s). Published by Elsevier B.V. on behalf of Research Network of Computational and Structural Biotechnology.

**Accession Number:** WOS:000607730700006

**PubMed ID:** 32637047

**ISSN:** 2001-0370

**Record 228 of 236**

**Title:** An In-Sight Into How Compression Dictionary Architecture Can Affect the Overall Performance in FPGAs

**Author(s):** Bartik, M (Bartik, Matej); Benes, T (Benes, Tomas); Kubalik, P (Kubalik, Pavel)

**Source:** IEEE ACCESS **Volume:** 8 **Pages:** 183101-183116 **DOI:** 10.1109/ACCESS.2020.3029691 **Published:** 2020

**Abstract:** This paper presents a detailed analysis of various approaches to hardware implemented compression algorithm dictionaries, including our optimized method. To obtain comprehensive and detailed results, we introduced a method for the fair comparison of programmable hardware architectures to show the benefits of our approach from the perspective of logic resources, frequency, and latency. We compared two generally used methods with our optimized method, which was found to be more suitable for maintaining the memory content via (in)valid bits in any mid-density memory structures, which are implemented in programmable hardware such as FPGAs (Field Programmable Gate Array). The benefits of our new method based on a x201C;Distributed Memoryx201D; technique are shown on a particular example of compression dictionary but the method is also suitable for another use cases requiring a fast (re-)initialization of the used memory structures before each run of an algorithm with minimum time and logic resources consumption. The performance evaluation of the respective approaches has been made in Xilinx ISE and Xilinx Vivado toolkits for the Virtex-7 FPGA family. However the proposed approach is compatible with 99x0025; of modern FPGAs.

**Accession Number:** WOS:000582655900001

**ISSN:** 2169-3536

**Record 229 of 236**

**Title:** Magnetism and magnetic anisotropy in UGa2

**Author(s):** Chatterjee, B (Chatterjee, Banhi); Koloenc, J (Koloenc, Jindrich)

**Source:** MRS ADVANCES **Volume:** 5 **Issue:** 51 **Special Issue:** SI **Pages:** 2639-2645 **DOI:** 10.1557/adv.2020.314 **Published:** 2020

**Abstract:** We investigate whether first-principles calculations with an improved description of electronic correlations can explain the large magnetic moments and the strong magnetocrystalline anisotropy in the ferromagnetic compound UGa2. The correlations are treated within a static mean-field approximation DFT+U combining the density functional theory (DFT) with an onsite Hubbard interaction U. We find that DFT+U improves the agreement of the magnetic moments with the experiment compared to DFT but worsens the theoretical description of the magnetocrystalline anisotropy.

**Accession Number:** WOS:000581816200004

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Chatterjee, Banhi		0000-0003-3032-6717
Koloenc, Jindrich	G-5405-2014	0000-0003-2627-8302

**ISSN:** 2059-8521

**Record 230 of 236**

**Title:** Scope and Application of Bi-Directional EDFA for long distance optical transmissions

**Author(s):** Bhowmick, S (Bhowmick, Sarbojeet); Vojtech, J (Vojtech, Josef); Velc, R (Velc, Radek)

**Edited by:** Kalli K; Peterka P; Bunge CA

**Source:** MICRO-STRUCTURED AND SPECIALTY OPTICAL FIBRES VI **Book Series:** Proceedings of SPIE **Volume:** 11355 **Article Number:** 113550P **DOI:** 10.1117/12.2553474 **Published:** 2020

**Abstract:** Erbium-Doped Fibre Amplifiers (EDFAs) caused a boom in optical communications world by allowing further possibilities of optical amplification without any O-E-O conversions, also in long haul transmission with number of channels simultaneously with other advanced transmissions (sensing, precise time and frequency transfers, etc.). EDFAs are used as a booster, [Mine, and pre-amplifier in an optical transmission system providing gain for signals either in C-Band or L-Band, or their edge. When the EDFA is being pumped at certain wavelength, Er ion doped in the fibre absorbs the pump light heading to an excited state. Amplification is achieved by ion de-excitation via stimulated emission and such phenomena have been used since 1980s. Generally, unidirectional solutions in fibre pairs for transmissions are preferred in telco field, as technically easier. Yet, we have large experience with the costs of leased fibres, and often bidirectional transmission in single fibre means savings for fibre leasing [1], and also often enables more than sufficient capacity in National Research and Education Network (NREN) environment. [2] And, bidirectional solutions in single fibre provide benefits for very advanced services, mostly Time and Frequency (T&F) transfers where only bidirectional transmission allows the highest precision. Single path bidirectional transmission is used in order to compensate thermal fluctuations, and provides the same length of both directions, which is crucial for T&F service. In this paper, we propagate bidirectional transmission measuring specifically over 1570nm wavelength. In our project, the tunable laser uses more efficient technique to attain an ultra-stable frequency gain rather than using ubiquitous ways in the optical network services.

**Accession Number:** WOS:000576761300016

**Conference Title:** Conference on Micro-Structured and Specialty Optical Fibres VI

**Conference Date:** APR 06-10, 2020

**Conference Location:** ELECTR NETWORK

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#### Record 231 of 236

**Title:** Intraspecific differentiation of *Sparganium erectum* in the Czech Republic: molecular, genome size and morphometric analysis

**Author(s):** Pisova, S (Pisova, Sonja); Fer, T (Fer, Tomas)

**Source:** PRESLIA Volume: 92 Issue: 2 Pages: 137-165 DOI: 10.23855/preslia.2020.137 Published: 2020

**Abstract:** Aquatic and wetland plants tend to be very phenotypically plastic, which accounts for the taxonomic difficulties in many groups. In the genus *Sparganium*, which comprises about 14 species, numerous taxa at different ranks are described. The classification of the genus is based on generative characters on the fruit, which are less influenced by the environment than vegetative characters. Nevertheless, the intraspecific division of *Sparganium erectum* poses problems, especially the existence of several intraspecific taxa along with intermediate individuals. In this study we examined four European subspecies of *S. erectum* (subsp. *erectum*, subsp. *microcarpum*, subsp. *neglectum* and subsp. *oocarpum*) from 64 populations in the Czech Republic. A combination of multivariate morphometrics, AFLPs and genome size estimation allowed us to confirm the current subspecies classification and investigate putative intraspecific hybridization. Four genetic groups with different genome sizes corresponding to the subspecies were found. Morphological characters that were described in previous studies correlated with these genetic groups and thus affirmed the classification. The most important characters for subspecies differentiation were width and length of fruit, style length, length of the upper part of the fruit and constriction in the middle part of the fruit. In addition, admixed individuals between the genetic groups were recorded. The hybrid origin of subsp. *oocarpum* was confirmed, being derived from the crossing of subsp. *erectum* and subsp. *neglectum*. Finally, three other hybrid combinations were detected, suggesting recent hybridization: subsp. *erectum* x subsp. *microcarpum*, subsp. *microcarpum* x subsp. *neglectum*, and subsp. *erectum* x subsp. *oocarpum*.

**Accession Number:** WOS:000573572400003

ISSN: 0032-7786

#### Record 232 of 236

**Title:** Improving RNN-based Answer Selection for Morphologically Rich Languages

**Author(s):** Medved, M (Medved, Marek); Sabol, R (Sabol, Radoslav); Horak, A (Horak, Ales)

**Edited by:** Rocha AP; Steels L; VanDenHerik J

**Source:** ICAART: PROCEEDINGS OF THE 12TH INTERNATIONAL CONFERENCE ON AGENTS AND ARTIFICIAL INTELLIGENCE, VOL 2 Pages: 644-651 DOI:

10.5220/0008979206440651 Published: 2020

**Abstract:** Question answering systems have improved greatly during the last five years by employing architectures of deep neural networks such as attentive recurrent networks or transformer-based networks with pretrained contextual information. In this paper, we present the results and detailed analysis of experiments with the largest question answering benchmark dataset for the Czech language. The best results evaluated in the text reach the accuracy of 72 %, which is a 4% improvement to the previous best result. We also introduce the newest version of the Czech Question Answering benchmark dataset SQUAD 3.0, which was substantially extended to more than 13,000 question-answer pairs, and we report the first answer selection results on this dataset which indicate that the size of the training data is important for the task.

**Accession Number:** WOS:000570769000069

**Conference Title:** 12th International Conference on Agents and Artificial Intelligence (ICAART)

**Conference Date:** FEB 22-24, 2020

**Conference Location:** Valletta, MALTA

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#### Record 233 of 236

**Title:** EFFECT OF Lambda PARTICLE PHONON COUPLING ON THE ENERGY SPECTRA OF He-5(Lambda) AND O-17(Lambda)

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

**Source:** ACTA PHYSICA POLONICA B Volume: 51 Issue: 3 Pages: 617-622 DOI: 10.5506/APhysPolB.51.617 Published: 2020

**Abstract:** The energy spectra of the hypernuclei He-5(Lambda) and O-17(Lambda) were studied within a multiphonon scheme, where the Lambda particle is coupled to particle-hole Tamm-Dancoff phonons describing the excitations of the core. A chiral interaction was used. The calculations show that the core excitations push considerably, through their coupling, the Hartree-Fock energies down in energy and enrich the low-energy spectrum in O-17(Lambda)

**Accession Number:** WOS:000521823800010

**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290

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#### Record 234 of 236

**Title:** NATURAL ORBITALS FOR THE EQUATION OF MOTION PHONON METHOD

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

**Source:** ACTA PHYSICA POLONICA B Volume: 51 Issue: 3 Pages: 623-630 DOI: 10.5506/APhysPolB.51.623 Published: 2020

**Abstract:** We discuss the use of natural orbitals as single-particle basis states for the Equation of Motion Phonon Method (EMPM). They are obtained by computing a ground-state one-body density matrix in second-order many-body perturbation theory. We focus our attention on energy and proton point radius of O-16 and show that, with respect to Hartree-Fock, the new basis improves drastically the convergence of the two-phonon correlation energy.

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#### Record 235 of 236

**Title:** Alternative spectral window for precise time fiber based transport

**Author(s):** Vojtech, J (Vojtech, Josef); Smotlacha, V (Smotlacha, Vladimir); Bhowmick, S (Bhowmick, Sarbojeet); Havlis, O (Havlis, Ondrej); Slapak, M (Slapak, Martin); Vohnout, R (Vohnout, Rudolf); Munster, P (Munster, Petr); Horvath, T (Horvath, Tomas); Velc, R (Velc, Radek); Kundrat, J (Kundrat, Jan); Altmannova, L (Altmannova, Lada); Michal, M (Michal, Martin); Skoda, P (Skoda, Pavel); Hazlinsky, M (Hazlinsky, Michal); Kubernat, V (Kubernat, Vaclav); Slavik, R (Slavik, Radan); Roztocil, J (Roztocil, Jaroslav)

**Book Group Author(s):** Inst Navigat

**Source:** PROCEEDINGS OF THE 51ST ANNUAL PRECISE TIME AND TIME INTERVAL SYSTEMS AND APPLICATIONS MEETING Book Series: Annual Precise Time and Time Interval Systems and Applications Meeting Pages: 187-190 Article Number: 17313 DOI: 10.33012/2020.17313 Published: 2020

**Abstract:** Precise time and also stable frequency transfers are approaching the state to become almost standard applications for optical fiber networks, especially they are becoming supported in multiple research and education networks. In principle, the time and frequency transfers are not possible to be implemented over data transport layer, which hasn't been designed for essential stability, and thus dedicated wave band is required for such implementation. To achieve even better stability for precise time and stable frequency, the bidirectional transmission in single physical medium (fibers and ideally all components along the route) is preferred. The White Rabbit system combines synchronous Ethernet and Precise Time Protocol (IEEE-1588) and it has been designed in the CERN with the aim to provide time synchronization among large number of sensors, actuators and other devices utilized in experiments. Primary aim was the operation over single fiber (to avoid nonreciprocal changes in directions) using standard telecommunication transceivers designed for single fiber operation with reach limited to about 40 km. In this paper, we experimentally verify and compare stability of White Rabbit system operation over long distances up to 300 km using active optical amplification on wavelengths which should not be utilized within spectrum needed for regular data transmissions.

**Accession Number:** WOS:000544823000006

**Conference Title:** 51st Annual Precise Time and Time Interval Systems and Applications Meeting

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**Conference Location:** San Diego, CA

**Conference Sponsors:** Inst Navigat

**Author Identifiers:**



Author	Web of Science ResearcherID	ORCID Number
Vohnout, Rudolf	O-7365-2019	0000-0002-6809-7377
Roztocil, Jaroslav		0000-0002-1795-4359
Slapak, Martin		0000-0002-7926-1398

ISSN: 2333-2085

**Record 236 of 236****Title:** Analysis of Hannan consistent selection for Monte Carlo tree search in simultaneous move games**Author(s):** Kovarik, V (Kovarik, Vojtech); Lisy, V (Lisy, Viliam)**Source:** MACHINE LEARNING **Volume:** 109 **Issue:** 1 **Pages:** 1-50 **DOI:** 10.1007/s10994-019-05832-z **Published:** JAN 2020

**Abstract:** Hannan consistency, or no external regret, is a key concept for learning in games. An action selection algorithm is Hannan consistent (HC) if its performance is eventually as good as selecting the best fixed action in hindsight. If both players in a zero-sum normal form game use a Hannan consistent algorithm, their average behavior converges to a Nash equilibrium of the game. A similar result is known about extensive form games, but the played strategies need to be Hannan consistent with respect to the counterfactual values, which are often difficult to obtain. We study zero-sum extensive form games with simultaneous moves, but otherwise perfect information. These games generalize normal form games and they are a special case of extensive form games. We study whether applying HC algorithms in each decision point of these games directly to the observed payoffs leads to convergence to a Nash equilibrium. This learning process corresponds to a class of Monte Carlo Tree Search algorithms, which are popular for playing simultaneous-move games but do not have any known performance guarantees. We show that using HC algorithms directly on the observed payoffs is not sufficient to guarantee the convergence. With an additional averaging over joint actions, the convergence is guaranteed, but empirically slower. We further define an additional property of HC algorithms, which is sufficient to guarantee the convergence without the averaging and we empirically show that commonly used HC algorithms have this property.

**Accession Number:** WOS:000512049900001**Author Identifiers:**

Author	Web of Science ResearcherID	ORCID Number
Kovarik, Vojtech	N-5407-2017	0000-0002-7954-9420

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