Record 1 of 274

Title: Altermagnetic lifting of Kramers spin degeneracy

Author(s): Krempasky, J (Krempasky, J.); Smejkal, L (Smejkal, L.); D'Souza, SW (D'Souza, S. W.); Hajlaoui, M (Hajlaoui, M.); Springholz, G (Springholz, G.); Uhlírová, K (Uhlirova, K.); Alarab, F (Alarab, F.); Constantinou, PC (Constantinou, P. C.); Strocov, V (Strocov, V.); Usanov, D (Usanov, D.); Pudelko, WR (Pudelko, W. R.); González-Hernández, R (Gonzalez-Hernandez, R.); Hellenes, AB (Hellenes, A. Birk); Jansa, Z (Jansa, Z.); Reichlová, H (Reichlova, H.); Sobán, Z (Soban, Z.); Betancourt, RDG (Betancourt, R. D. Gonzalez); Wadley, P (Wadley, P.); Sinova, J (Sinova, J.); Kriegner, D (Kriegner, D.); Minár, J (Minar, J.); Dil, JH (Dil, J. H.); Jungwirth, T (Jungwirth, T.)

Source: NATURE **Volume:** 626 **Issue:** 7999 **Pages:** 517-+ **DOI:** 10.1038/s41586-023-06907-7 **Published Date:** 2024 FEB 15

Abstract: Lifted Kramers spin degeneracy (LKSD) has been among the central topics of condensed-matter physics since the dawn of the band theory of solids(1,2). It underpins established practical applications as well as current frontier research, ranging from magnetic-memory technology(3-7) to topological quantum matter(8-14). Traditionally, LKSD has been considered to originate from two possible internal symmetry-breaking mechanisms. The first refers to time-reversal symmetry breaking by magnetization of ferromagnets and tends to be strong because of the non-relativistic exchange origin(15). The second applies to crystals with broken inversion symmetry and tends to be comparatively weaker, as it originates from the relativistic spin-orbit coupling (SOC)(16-19). A recent theory work based on spin-symmetry classification has identified an unconventional magnetic phase, dubbed altermagnetic(20,21), that allows for LKSD without net magnetization and inversion-symmetry breaking. Here we provide the confirmation using photoemission spectroscopy and ab initio calculations. We identify two distinct unconventional mechanisms of LKSD generated by the altermagnetic phase of centrosymmetric MnTe with vanishing net magnetization(20-23). Our observation of the altermagnetic LKSD can have broad consequences in magnetism. It motivates exploration and exploitation of the unconventional nature of this magnetic phase in an extended family of materials, ranging from insulators and semiconductors to metals and superconductors(20,21), that have been either identified recently or perceived for many decades as conventional antiferromagnets(21,24,25).

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Record 2 of 274

Title: X-ray eruptions every 22 days from the nucleus of a nearby galaxy

Author(s): Guolo, M (Guolo, Muryel); Pasham, DR (Pasham, Dheeraj R.); Zajacek, M (Zajacek, Michal); Coughlin, ER (Coughlin, Eric R.); Gezari, S (Gezari, Suvi); Suková, P (Sukova, Petra); Wevers, T (Wevers, Thomas); Witzany, V (Witzany, Vojtech); Tombesi, F (Tombesi, Francesco); van Velzen, S (van Velzen, Sjoert); Alexander, KD (Alexander, Kate D.); Yao, YH (Yao, Yuhan); Arcodia, R (Arcodia, Riccardo); Karas, V (Karas, Vladimir); Miller-Jones, JCA (Miller-Jones, James C. A.); Remillard, R (Remillard, Ronald); Gendreau, K (Gendreau, Keith); Ferrara, EC (Ferrara, Elizabeth C.)

Source: NATURE ASTRONOMY **Volume:** 8 **Issue:** 3 **DOI:** 10.1038/s41550-023-02178-4 **Early Access Date:** JAN 2024 **Published Date:** 2024 MAR

Abstract: Galactic nuclei showing recurrent phases of activity and quiescence have recently been discovered. Some have recurrence times as short as a few hours to a day and are known as quasi-periodic X-ray eruption (QPE) sources. Others have recurrence times as long as hundreds to a thousand days and are called repeating nuclear transients. Here we present a multiwavelength overview of Swift J023017.0+283603 (hereafter Swift J0230+28), a source from which repeating and quasi-periodic X-ray flares are emitted from the nucleus of a previously unremarkable galaxy at similar to 165 Mpc. It has a recurrence time of approximately 22 days, an intermediary timescale between known repeating nuclear transients and QPE sources. The source also shows transient radio emission, likely associated with the X-ray emission. Such recurrent soft X-ray eruptions, with no accompanying ultraviolet or optical emission, are strikingly similar to QPE sources. However, in addition to having a recurrence time that is similar to 25 times longer than the longest-known QPE source, Swift J0230+28's eruptions exhibit somewhat distinct shapes and temperature evolution compared to the known QPE sources. Scenarios involving extreme mass ratio inspirals are favoured over disk instability models. The source reveals an unexplored timescale for repeating extragalactic transients and highlights the need for a wide-field, time-domain X-ray mission to explore the parameter space of recurring X-ray transients.
Multiwavelength observations of a galactic nucleus exhibit quasi-periodic X-ray eruptions (QPEs) that repeat every 22 days, a timescale intermediate between those of other QPEs and so-called repeating nuclear transients. The eruptions are likely to be driven by the interaction between an orbiting body and a central massive black hole.

Accession Number: WOS:001141914300001

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Record 3 of 274

Title: X-Ray Magnetic Circular Dichroism in Altermagnetic α-MnTe

Author(s): Hariki, A (Hariki, A.); Dal Din, A (Dal Din, A.); Amin, OJ (Amin, O. J.); Yamaguchi, T (Yamaguchi, T.); Badura, A (Badura, A.); Kriegner, D (Kriegner, D.); Edmonds, KW (Edmonds, K. W.); Campion, RP (Campion, R. P.); Wadley, P (Wadley, P.); Backes, D (Backes, D.); Veiga, LSI (Veiga, L. S. I.); Dhesi, SS (Dhesi, S. S.); Springholz, G (Springholz, G.); Smejkal, L (Smejkal, L.); Vyborny, K (Vyborny, K.); Jungwirth, T (Jungwirth, T.); Kune, J (Kune, J.)

Source: PHYSICAL REVIEW LETTERS **Volume:** 132 **Issue:** 17 **Article Number:** 176701 **DOI:** 10.1103/PhysRevLett.132.176701 **Published Date:** 2024 APR 23

Abstract: Altermagnetism is a recently identified magnetic symmetry class combining characteristics of conventional collinear ferromagnets and antiferromagnets, that were regarded as mutually exclusive, and enabling phenomena and functionalities unparalleled in either of the two traditional elementary magnetic classes. In this work we use symmetry, ab initio theory, and experiments to explore x-ray magnetic circular dichroism (XMCD) in the altermagnetic class. As a representative material for our XMCD study we choose alpha-MnTe with compensated antiparallel magnetic order in which an anomalous Hall effect has been already demonstrated. We predict and experimentally confirm a characteristic XMCD line shape for compensated moments lying in a plane perpendicular to the light propagation vector. Our results highlight the distinct phenomenology in altermagnets of this time-reversal symmetry breaking response, and its potential utility for element-specific spectroscopy and microscopy.

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PubMed ID: 38728732

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Record 4 of 274

Title: FireProt 2.0: web-based platform for the fully automated design of thermostable proteins

Author(s): Musil, M (Musil, Milos); Jezik, A (Jezik, Andrej); Horackova, J (Horackova, Jana); Borko, S (Borko, Simeon); Kabourek, P (Kabourek, Petr); Damborsky, J (Damborsky, Jiri); Bednar, D (Bednar, David)

Source: BRIEFINGS IN BIOINFORMATICS **Volume:** 25 **Issue:** 1 **Article Number:** bbad425 **DOI:** 10.1093/bib/bbad425 **Published Date:** 2024 JAN

Abstract: Thermostable proteins find their use in numerous biomedical and biotechnological applications. However, the computational design of stable proteins often results in single-point mutations with a limited effect on protein stability. However, the construction of stable multiple-point mutants can prove difficult due to the possibility of antagonistic effects between individual mutations. FireProt protocol enables the automated computational design of highly stable multiple-point mutants. FireProt 2.0 builds on top of the previously published FireProt web, retaining the original functionality and

expanding it with several new stabilization strategies. FireProt 2.0 integrates the AlphaFold database and the homology modeling for structure prediction, enabling calculations starting from a sequence. Multiple-point designs are constructed using the Bron-Kerbosch algorithm minimizing the antagonistic effect between the individual mutations. Users can newly limit the FireProt calculation to a set of user-defined mutations, run a saturation mutagenesis of the whole protein or select rigidifying mutations based on B-factors. Evolution-based back-to-consensus strategy is complemented by ancestral sequence reconstruction. FireProt 2.0 is significantly faster and a reworked graphical user interface broadens the tool's availability even to users with older hardware. FireProt 2.0 is freely available at http://loschmidt.chemi.muni.cz/fireprotweb.

Accession Number: WOS:001173375300007

PubMed ID: 38018911

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ISSN: 1467-5463

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Record 5 of 274

Title: On-Surface Synthesis and Determination of the Open-Shell Singlet Ground State of Tridecacene

Author(s): Zuzak, R (Zuzak, Rafal); Kumar, M (Kumar, Manish); Stoica, O (Stoica, Otilia); Soler-Polo, D (Soler-Polo, Diego); Brabec, J (Brabec, Jiri); Pernal, K (Pernal, Katarzyna); Veis, L (Veis, Libor); Blieck, R (Blieck, Remi); Echavarren, AM (Echavarren, Antonio M.); Jelinek, P (Jelinek, Pavel); Godlewski, S (Godlewski, Szymon)

Source: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 63 **Issue:** 9 **DOI:** 10.1002/anie.202317091 **Early Access Date:** JAN 2024 **Published Date:** 2024 FEB 26

Abstract: The character of the electronic structure of acenes has been the subject of longstanding discussion. However, convincing experimental evidence of their open-shell character has so far been missing. Here, we present the on-surface synthesis of tridecacene molecules by thermal annealing of octahydrotridecacene on a Au(111) surface. We characterized the electronic structure of the tridecacene by scanning probe microscopy, which reveals the presence of an inelastic signal at 126 meV. We attribute the inelastic signal to spin excitation from the singlet diradical ground state to the triplet excited state. To rationalize the experimental findings, we carried out many-body ab initio calculations as well as model Hamiltonians to take into account the effect of the metallic substrate. Moreover, we provide a detailed analysis of how the dynamic electron correlation and virtual charge fluctuation between the molecule and metallic surface reduces the singlet-triplet band gap. Thus, this work provides the first experimental confirmation of the magnetic character of tridecacene.
Tridecacenes were synthesized on Au(111) and their properties were characterized by combined scanning tunneling spectroscopy, inelastic electron tunneling spectroscopy, and state-of-the-art many body calculations. The study confirmed the open-shell diradical character and demonstrated that the magnitude of the singlet-triplet band gap is affected by the proximity of the surface as well as a dynamic electron correlation.**+image

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PubMed ID: 38192200

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Record 6 of 274

Title: The fractional soliton solutions of dynamical system arising in plasma physics: The comparative analysis

Author(s): Faridi, WA (Faridi, Waqas Ali); Iqbal, M (Iqbal, Mujahid); Riaz, MB (Riaz, Muhammad Bilal); Alqahtani, SA (Alqahtani, Salman A.); Wazwaz, AM (Wazwaz, Abdul-Majid)

Source: ALEXANDRIA ENGINEERING JOURNAL **Volume:** 95 **Pages:** 247-261 **DOI:** 10.1016/j.aej.2024.03.061 **Early Access Date:** APR 2024 **Published Date:** 2024 MAY

Abstract: In light of fractional theory, this paper presents several new effective solitonic formulations for the Langmuir and ion sound wave equations. Prior to this study, no previous research has presented the comparision and obtained the generalized fractional soliton solutions of this kind with power law kernel and Mittag-Leffler kernel. The ion sound and Langmuir wave equations are essential in plasma physics, offering insights into the collective behavior of charged particles in plasmas and enabling diagnostics and control of these complex, ionized gas systems. The two distinct fractional order differential operators are substituted for the traditional order derivative to reshape the examined model. The Atangana-Baleanu non-singular and non -local operator and conformable fractional operator are the fractional -order operators that are used to create the fractional complex system equations for Langmuir waves and ion sound. A constructive approach new auxiliary equation method utilizes to obtain the exact analytical soliton solutions for ion sound and Langmuir wave equation. A wide range of soliton solutions is obtained, including mixed complex solitary shock solutions, singular solutions, mixed shock singular solutions, mixed trigonometric solutions, mixed singular solutions, exact solutions, mixed periodic solutions, and mixed hyperbolic solutions, dark soliton, bright soliton, trigonometric solutions, periodic results, and hyperbolic results. The solitons solution of the ion sound and Langmuir wave equations lies in their ability to maintain wave stability, their role in modeling wave propagation and nonlinear effects, their potential use as diagnostic tools, and their relevance in wave -particle interactions in plasma physics. The solitons provide a valuable framework for understanding the behavior of waves in plasmas and offer insights into the complex dynamics of these charged particle systems. A graphical comparison analysis of a few solutions is also shown here, taking into account appropriate parametric values through the use of the software package. Moreover, the results of this study have important implications for Hamilton's equations and generalized momentum, where solitons are employed in long-range interactions.

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Record 7 of 274

Title: Dimorphos Orbit Determination from Mutual Events Photometry

Author(s): Scheirich, P (Scheirich, Peter); Pravec, P (Pravec, Petr); Meyer, AJ (Meyer, Alex J.); Agrusa, HF (Agrusa, Harrison F.); Richardson, DC (Richardson, Derek C.); Chesley, SR (Chesley, Steven R.); Naidu, SP (Naidu, Shantanu P.); Thomas, C (Thomas, Cristina); Moskovitz, NA (Moskovitz, Nicholas A.)

Source: PLANETARY SCIENCE JOURNAL **Volume:** 5 **Issue:** 1 **Article Number:** 17 **DOI:** 10.3847/PSJ/ad12cf **Published Date:** 2024 JAN 1

Abstract: The NASA Double Asteroid Redirection Test spacecraft successfully impacted the Didymos-Dimorphos binary asteroid system on 2022 September 26 UTC. We provide an update to its preimpact mutual orbit and estimate the postimpact physical and orbital parameters, derived using ground-based photometric observations taken from 2022 July to 2023 February. We found that the total change of the orbital period was -33.240 +/- 0.072 minutes (all uncertainties are 3 sigma). We obtained the eccentricity of the postimpact orbit to be 0.028 +/- 0.016 and the apsidal precession rate was 7.3 +/- 2.0 degrees day-1 from the impact to 2022 December 2. The data taken later in 2022 December to 2023 February suggest that the eccentricity dropped close to zero or the orbit became chaotic approximately 70 days after the impact. Most of the period change took place immediately after the impact, but in the few weeks following the impact it was followed by an additional change of -27-58+19 s or -19 +/- 18 s (the two values depend on the approach we used to describe the evolution of the orbital period after the impact-an exponentially decreasing angular acceleration or the assumption of a constant orbital period, which changed abruptly some time after the impact, respectively). We estimate the preimpact Dimorphos-Didymos size ratio was 0.223 +/- 0.012 and the postimpact is 0.202 +/- 0.018, which indicate a marginally significant reduction of Dimorphos' volume by (9 +/- 9)% as the result of the impact.

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Record 8 of 274

Title: Submolecular-scale control of phototautomerization

Author(s): Roslawska, A (Roslawska, Anna); Kaiser, K (Kaiser, Katharina); Romeo, M (Romeo, Michelangelo); Devaux, E (Devaux, Eloise); Scheurer, F (Scheurer, Fabrice); Berciaud, S (Berciaud, Stephane); Neuman, T (Neuman, Tomas); Schull, G (Schull, Guillaume)

Source: NATURE NANOTECHNOLOGY **Volume:** 19 **Issue:** 6 **DOI:** 10.1038/s41565-024-01622-4 **Early Access Date:** FEB 2024 **Published Date:** 2024 JUN

Abstract: Optically activated reactions initiate biological processes such as photosynthesis or vision, but can also control polymerization, catalysis or energy conversion. Methods relying on the manipulation of light at macroscopic and mesoscopic scales are used to control on-surface photochemistry, but do not offer atomic-scale control. Here we take advantage of the confinement of the electromagnetic field at the apex of a scanning tunnelling microscope tip to drive the phototautomerization of a free-base phthalocyanine with submolecular precision. We can control the reaction rate and the relative tautomer population through a change in the laser excitation wavelength or through the tip position. Atomically resolved tip-enhanced photoluminescence spectroscopy and hyperspectral mapping unravel an excited-state mediated process, which is quantitatively supported by a comprehensive theoretical model combining ab initio calculations with a parametric open-quantum-system approach. Our experimental strategy may allow insights in other photochemical reactions and proof useful to control complex on-surface reactions.
Weak laser light confined at the apex of a scanning tunnelling microscope tip can drive the tautomerization of a free-base phthalocyanine with atomic-scale precision. The combination of tip-enhanced photoluminescence spectroscopy and hyperspectral mapping paired with theoretical modelling then unravel an excited-state mediated reaction.

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PubMed ID: 38413791

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Record 9 of 274

Title: Density functional theory methods applied to homogeneous and heterogeneous catalysis: a short review and a practical user guide

Author(s): Butera, V (Butera, Valeria)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 26 **Issue:** 10 **Pages:** 7950-7970 **DOI:** 10.1039/d4cp00266k **Early Access Date:** FEB 2024 **Published Date:** 2024 MAR 6

Abstract: The application of density functional theory (DFT) methods in catalysis has been growing fast in the last few decades thanks to both the availability of more powerful high computing resources and the development of new efficient approximations and approaches. DFT calculations allow for the understanding of crucial catalytic aspects that are difficult or even impossible to access by experiments, thus contributing to faster development of more efficient and selective catalysts. Depending on the catalytic system and properties under investigation, different approaches should be used. Moreover, the

reliability of the obtained results deeply depends on the approximations involved in both the selected method and model. This review addresses chemists, physicists and materials scientists whose interest deals with the application of DFT-based computational tools in both homogeneous catalysis and heterogeneous catalysis. First, a brief introduction to DFT is presented. Then, the main approaches based on atomic centered basis sets and plane waves are discussed, underlining the main differences, advantages and limitations. Eventually, guidance towards the selection of the catalytic model is given, with a final focus on the evaluation of the energy barriers, which represents a crucial step in all catalytic processes. Overall, the review represents a rational and practical guide for both beginners and more experienced users involved in the wide field of catalysis.
A rational and practical guide for the application of DFT methods in the wide field of catalysis.

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Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Butera, Valeria	JCE-4132-2023	

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Record 10 of 274

Title: Direct Laser Acceleration in Underdense Plasmas with Multi-PW Lasers: A Path to High-Charge, GeV-Class Electron Bunches

Author(s): Babjak, R (Babjak, R.); Willingale, L (Willingale, L.); Arefiev, A (Arefiev, A.); Vranic, M (Vranic, M.)

Source: PHYSICAL REVIEW LETTERS **Volume:** 132 **Issue:** 12 **Article Number:** 125001 **DOI:** 10.1103/PhysRevLett.132.125001 **Published Date:** 2024 MAR 22

Abstract: The direct laser acceleration (DLA) of electrons in underdense plasmas can provide hundreds of nC of electrons accelerated to near -GeV energies using currently available lasers. Here we demonstrate the key role of electron transverse displacement in the acceleration and use it to analytically predict the expected maximum electron energies. The energy scaling is shown to be in agreement with full-scale quasi -3D particle -in -cell simulations of a laser pulse propagating through a preformed guiding channel and can be directly used for optimizing DLA in near -future laser facilities. The strategy towards optimizing DLA through matched laser focusing is presented for a wide range of plasma densities paired with current and near -future laser technology. Electron energies in excess of 10 GeV are accessible for lasers at I - 1021 W/cm2.

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PubMed ID: 38579225

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Record 11 of 274

Title: Beyond the marrow: insights from comprehensive next-generation sequencing of extramedullary multiple myeloma tumors

Author(s): Jelinek, T (Jelinek, T.); Zihala, D (Zihala, D.); Sevcikova, T (Sevcikova, T.); Sithara, AA (Anilkumar Sithara, A.); Kapustova, V (Kapustova, V.); Sahinbegovic, H (Sahinbegovic, H.); Venglar, O (Venglar, O.); Muronova, L (Muronova, L.); Broskevicova, L (Broskevicova, L.); Nenarokov, S (Nenarokov, S.); Bilek, D (Bilek, D.); Popkova, T (Popkova, T.); Plonkova, H (Plonkova, H.); Vrana, J (Vrana, J.); Zidlik, V (Zidlik, V.); Hurnik, P (Hurnik, P.); Havel, M (Havel, M.); Hrdinka, M (Hrdinka, M.); Chyra, Z (Chyra, Z.); Stracquadanio, G (Stracquadanio, G.); Simicek, M (Simicek, M.); Hajek, R (Hajek, R.)

Source: LEUKEMIA **Volume:** 38 **Issue:** 6 **Pages:** 1323-1333 **DOI:** 10.1038/s41375-024-02206-w **Early Access Date:** MAR 2024 **Published Date:** 2024 JUN

Abstract: Extramedullary multiple myeloma (EMM) is an aggressive form of multiple myeloma (MM). This study represents the most comprehensive next-generation sequencing analysis of EMM tumors (N = 14) to date, uncovering key molecular features and describing the tumor microenvironment. We observed the co-occurrence of 1q21 gain/amplification and MAPK pathway mutations in 79% of EMM samples, suggesting that these are crucial mutational events in EMM development. We also demonstrated that patients with mutated KRAS and 1q21 gain/amplification at the time of diagnosis have a significantly higher risk of EMM development (HR = 2.4, p = 0.011) using data from a large CoMMpass dataset. We identified downregulation of CXCR4 and enhanced cell proliferation, along with reduced expression of therapeutic targets (CD38, SLAMF7, GPRC5D, FCRH5), potentially explaining diminished efficacy of immunotherapy. Conversely, we identified significantly upregulated EZH2 and CD70 as potential future therapeutic options. For the first time, we report on the tumor microenvironment of EMM, revealing CD8+ T cells and NK cells as predominant immune effector cells using single-cell sequencing. Finally, this is the first longitudinal study in EMM revealing the molecular changes from the time of diagnosis to EMM relapse.

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Record 12 of 274

Title: The anti-aromatic dianion and aromatic tetraanion of [18]annulene

Author(s): Stawski, W (Stawski, Wojciech); Zhu, YK (Zhu, Yikun); Roncevic, I (Roncevic, Igor); Wei, Z (Wei, Zheng); Petrukhina, MA (Petrukhina, Marina A.); Anderson, HL (Anderson, Harry L.)

Source: NATURE CHEMISTRY **Volume:** 16 **Issue:** 6 **DOI:** 10.1038/s41557-024-01469-1 **Early Access Date:** MAR 2024 **Published Date:** 2024 JUN

Abstract: pi-Conjugated macrocycles behave differently from analogous linear chains because their electronic wavefunctions resemble a quantum particle on a ring, leading to aromaticity or anti-aromaticity. [18]Annulene, (CH)18, is the archetypal non-benzenoid aromatic hydrocarbon. Molecules with circuits of 4n + 2 pi electrons, such as [18]annulene (n = 4), are aromatic, with enhanced stability and diatropic ring currents (magnetic shielding inside the ring), whereas those with 4n pi electrons, such as the dianion of [18]annulene, are expected to be anti-aromatic and exhibit the opposite behaviour. Here we use 1H NMR spectroscopy to re-evaluate the structure of the [18]annulene dianion. We also show that it can be reduced further to an aromatic tetraanion, which has the same shape as the dianion. The crystal structure of the tetraanion lithium salt confirms its geometry and reveals a metallocene-like sandwich, with five Li+ cations intercalated between two [18]annulene tetraanions. We also report a heteroleptic sandwich, with [18]annulene and corannulene tetraanion decks.
A previous investigation of the anti-aromatic dianion of [18]annulene concluded that it consists of a mixture of two isomers. Now it has been shown that this dianion exists as a single isomer, with a different geometry from neutral [18]annulene, and that it can be reduced further to an aromatic tetraanion.

Accession Number: WOS:001179908800001

PubMed ID: 38448656

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Record 13 of 274

Title: The odd-number cyclo[13]carbon and its dimer, cyclo[26]carbon

Author(s): Albrecht, F (Albrecht, Florian); Roncevic, I (Roncevic, Igor); Gao, YZ (Gao, Yueze); Paschke, F (Paschke, Fabian); Baiardi, A (Baiardi, Alberto); Tavernelli, I (Tavernelli, Ivano); Mishra, S (Mishra, Shantanu); Anderson, HL (Anderson, Harry L.); Gross, L (Gross, Leo)

Source: SCIENCE **Volume:** 384 **Issue:** 6696 **Pages:** 677-682 **DOI:** 10.1126/science.ado1399 **Published Date:** 2024 MAY 10

Abstract: Molecular rings of N carbon atoms (cyclo[N]carbons, or C-N) are excellent benchmarking systems for testing quantum chemical theoretical methods and valuable precursors to other carbon-rich materials. Odd-N cyclocarbons, which have been elusive to date, are predicted to be even less stable than even-N cyclocarbons. We report the on-surface synthesis of cyclo[13]carbon, C-13, by manipulation of decachlorofluorene with a scanning probe microscope tip. We elucidated the properties of C-13 by experiment and theoretical modeling. C-13 adopts an open-shell configuration with a triplet ground state and a kinked geometry, which shows different extents of distortion and carbene localization depending on the molecular environment. Moreover, we prepared and characterized the C-13 dimer, cyclo[26]carbon, demonstrating the potential of cyclocarbons and their precursors as building blocks for carbon allotropes.

Accession Number: WOS:001253561400014

PubMed ID: 38723091

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ISSN: 0036-8075

eISSN: 1095-9203

Record 14 of 274

Title: New mass-loss rates of Magellanic Cloud B supergiants from global wind models

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

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 681 **Article Number:** A29 **DOI:** 10.1051/0004-6361/202347916 **Published Date:** 2024 JAN 3

Abstract: We provide global models of line-driven winds of B supergiants for metallicities corresponding to the Large and Small Magellanic Clouds. The velocity and density structure of the models is determined consistently from hydrodynamical equations with radiative force derived in the comoving frame and level populations computed from kinetic equilibrium equations. We provide a formula expressing the predicted mass-loss rates in terms of stellar luminosity, effective temperature, and metallicity. Predicted wind mass-loss rates decrease with decreasing metallicity as (M) over dot similar to Z(0.60) and are proportional to the stellar luminosity. The mass-loss rates increase below the region of the bistability jump at about 20 kK because of iron recombination. In agreement with previous theoretical and observational studies, we find a smooth change of wind properties in the region of the bistability jump. With decreasing metallicity, the bistability jump becomes weaker and shifts to lower effective temperatures. At lower metallicities above the bistability jump, our predictions provide similar rates to those used in current evolutionary models, but our rates are significantly lower than older predictions below the bistability jump. Our predicted mass-loss rates agree with observational estimates derived from H alpha line assuming that observations of stellar winds from Galaxy and the Magellanic Clouds are uniformly affected by clumping. The models nicely reproduce the dependence of terminal velocities on temperature derived from ultraviolet spectroscopy.

Accession Number: WOS:001135685000003

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ISSN: 0004-6361

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Record 15 of 274

Title: Evaluating energy transmission characteristics of Non-Newtonian fluid flow in stratified and non-stratified regimes: A comparative study

Author(s): Bilal, S (Bilal, S.); Asadullah (Asadullah); Riaz, MB (Riaz, Muhammad Bilal)

Source: RESULTS IN ENGINEERING **Volume:** 22 **Article Number:** 102157 **DOI:** 10.1016/j.rineng.2024.102157 **Early Access Date:** MAY 2024 **Published Date:** 2024 JUN

Abstract: Considering the natural and industrial importance of flow characterization in stratified media, the current study is articulated. This work highlights the influence of linear stratification as well as convective surfaces in both thermal and solutal fields on the rheological attributes of Williamson fluid flow through an inclined surface. Novel physical aspects of a uniformly provided magnetic field of strength B and chemically reactive species are also included. The concerned transport equations are derived from the associated conservation laws in dimensional forms. Modification in the developed couple system is achieved by using a set of similar variables. Levenberg-Marquardt Scheme (LMS) and Bayesian Regularization Scheme (BRS) are utilized in comparative manner to analyze initial data accessed for quantities of interest. The data used in the generation of MLP was 80 percent for model training and 20 percent for testing and validation. Error histograms, performance plots, fitness curves, and regression plots for training, testing, and validation are presented. Data in the form of tables and graphs are presented, which express an excellent match between the ANN-predicted and targeted values. It is revealed that an artificial neural network approach can provide highly efficient forecasting for such problems by providing accurate data for quantities of interest. It is noticed that Nusselt number and Sherwood number enhances up to 33 % and 29 % versus respective stratification parameters. Velocity profile declines against magnetic field parameter (M) whereas, skin friction coefficient increments up to 25 %. Appliance of convective boundary constraints at the surface of inclined sheet tends to enhance the temperature and concentration fields.

Accession Number: WOS:001239444300001

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ISSN: 2590-1230

Record 16 of 274

Title: The transcriptome landscape of developing <break/>barley seeds

Author(s): Kovacik, M (Kovacik, Martin); Nowicka, A (Nowicka, Anna); Zwyrtková, J (Zwyrtkova, Jana); Strejcková, B (Strejckova, Beata); Vardanega, I (Vardanega, Isaia); Esteban, E (Esteban, Eddi); Pasha, A (Pasha, Asher); Kaduchová, K (Kaduchova, Katerina); Krautsova, M (Krautsova, Maryna); Cervenková, M (Cervenkova, Marie); Safár, J (Safar, Jan); Provart, NJ (Provart, Nicholas J.); Simon, R (Simon, Ruediger); Pecinka, A (Pecinka, Ales)

Source: PLANT CELL **Volume:** 36 **Issue:** 7 **Pages:** 2512-2530 **DOI:** 10.1093/plcell/koae095 **Early Access Date:** APR 2024 **Published Date:** 2024 APR 18

Abstract: Cereal grains are an important source of food and feed. To provide comprehensive spatiotemporal information about biological processes in developing seeds of cultivated barley (Hordeum vulgare L. subsp. vulgare), we performed a transcriptomic study of the embryo, endosperm, and seed maternal tissues collected from grains 4-32 days after pollination. Weighted gene co-expression network and motif enrichment analyses identified specific groups of genes and transcription factors (TFs) potentially regulating barley seed tissue development. We defined a set of tissue-specific marker genes and families of TFs for functional studies of the pathways controlling barley grain development. Assessing selected groups of chromatin regulators revealed that epigenetic processes are highly dynamic and likely play a major role during barley endosperm development. The repressive H3K27me3 modification is globally reduced in endosperm tissues and at specific genes related to development and storage compounds. Altogether, this atlas uncovers the complexity of developmentally regulated gene expression in developing barley grains.

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PubMed ID: 38635902

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ISSN: 1040-4651

eISSN: 1532-298X

Record 17 of 274

Title: Novel numerical approach toward hybrid nanofluid flow subject to Lorentz force and homogenous/heterogeneous chemical reaction across coaxial cylinders

Author(s): Janjua, KH (Janjua, Khuram Hina); Bilal, M (Bilal, Muhammad); Riaz, MB (Riaz, Muhammad Bilal); Saqib, AB (Saqib, Abdul Baseer); Ismail, EAA (Ismail, Emad A. A.); Awwad, FA (Awwad, Fuad A.)

Source: AIP ADVANCES **Volume:** 14 **Issue:** 7 **Article Number:** 075129 **DOI:** 10.1063/5.0214594 **Published Date:** 2024 JUL 1

Abstract: The combination of AA7075 and Ti6Al4V aluminum alloys provides an effective balance of endurance, corrosion resistance, and lightness. Some potential applications include aviation components, marine structures with anti-corrosion characteristics, surgical instruments, and athletic apparel. Therefore, the hybrid nanofluid (Hnf) consists of aluminum alloys (AA7075-Ti6Al4V), water (50%), and ethylene glycol (EG-50%) in the current analysis. The Hnf flow subject to heat radiation and Lorentz force is studied through coaxial cylinders. In addition, the flow has been observed under the impacts of homogeneous-heterogeneous (HH) chemical reaction and exponential heat source/sink. The modeled equations (continuity, momentum, HH, and heat equations) are renovated into the non-dimensional form through the similarity approach, which are further numerically computed by employing the ND-solve technique coupling with the shooting method. It can be noticed from the graphical results that the flow rate of Hnf drops with the rising effect of porosity and magnetic field parameters. The addition of AA7075-Ti6Al4V nanoparticles (NPs) also reduces the fluid temperature and velocity profile. Furthermore, the concentration distribution diminishes with the flourishing effect of HH parameters.

Accession Number: WOS:001280629300001

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eISSN: 2158-3226

Record 18 of 274

Title: The LOFAR Two-metre Sky Survey: The nature of the faint source population and SFR-radio luminosity relation using PROSPECTOR

Author(s): Das, S (Das, Soumyadeep); Smith, DJB (Smith, Daniel J. B.); Haskell, P (Haskell, Paul); Hardcastle, MJ (Hardcastle, Martin J.); Best, PN (Best, Philip N.); Duncan, KJ (Duncan, Kenneth J.); Arnaudova, M (Arnaudova, Marina, I); Shenoy, S (Shenoy, Shravya); Kondapally, R (Kondapally, Rohit); Cochrane, RK (Cochrane, Rachel K.); Drake, AB (Drake, Alyssa B.); Gürkan, G (Gurkan, Gulay); Malek, K (Malek, Katarzyna); Morabito, LK (Morabito, Leah K.); Prandoni, I (Prandoni, Isabella)

Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY **Volume:** 531 **Issue:** 1 **Pages:** 977-996 **DOI:** 10.1093/mnras/stae1204 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 13

Abstract: Spectral energy distribution (SED) fitting has been extensively used to determine the nature of the faint radio source population. Recent efforts have combined fits from multiple SED-fitting codes to account for the host galaxy and any active nucleus that may be present. We show that it is possible to produce similar-quality classifications using a single energy-balance SED fitting code, PROSPECTOR, to model up to 26 bands of UV-far-infrared aperture-matched photometry for similar to 31 000 sources in the ELAIS-N1 field from the LOFAR Two-Metre Sky Survey (LoTSS) deep fields first data release. One of a new generation of SED-fitting codes, PROSPECTOR accounts for potential contributions from radiative active galactic nuclei (AGN) when estimating galaxy properties, including star formation rates (SFRs) derived using non-parametric star formation histories. Combining this information with radio luminosities, we classify 92 per cent of the radio sources as a star-forming galaxy, high-/low-excitation radio galaxy, or radio-quiet AGN and study the population demographics as a function of 150 MHz flux density, luminosity, SFR, stellar mass, redshift, and apparent r-band magnitude. Finally, we use PROSPECTOR SED fits to investigate the SFR-150 MHz luminosity relation for a sample of similar to 133 000 3.6 mu m-selected $z < 1$ sources, finding that the stellar mass dependence is significantly weaker than previously reported, and may disappear altogether at $\log(10)(\mathrm{SFR}/\mathrm{M\text{-}circle\ dot\ yr}(-1)) > 0.5$. This approach makes it significantly easier to classify radio sources from LoTSS and elsewhere, and may have important implications for future studies of star-forming galaxies at radio wavelengths.

Accession Number: WOS:001227688600002

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ISSN: 0035-8711

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Record 19 of 274

Title: Insertases scramble lipids: Molecular simulations of MTCH2

Author(s): Bartos, L (Bartos, Ladislav); Menon, AK (Menon, Anant K.); Vácha, R (Vacha, Robert)

Source: STRUCTURE **Volume:** 32 **Issue:** 4 **DOI:** 10.1016/j.str.2024.01.012 **Early Access Date:** APR 2024 **Published Date:** 2024 APR 4

Abstract: Scramblases play a pivotal role in facilitating bidirectional lipid transport across cell membranes, thereby influencing lipid metabolism, membrane homeostasis, and cellular signaling. MTCH2, a mitochondrial outer membrane protein insertase, has a membrane -spanning hydrophilic groove resembling those that form the lipid transit pathway in known scramblases. Employing both coarse -grained and atomistic molecular dynamics simulations, we show that MTCH2 significantly reduces the free energy barrier for lipid movement along the groove and therefore can indeed function as a scramblase. Notably, the scrambling rate of MTCH2 in silico is similar to that of voltage -dependent anion channel (VDAC), a recently discovered scramblase of the outer mitochondrial membrane, suggesting a potential complementary physiological role for these mitochondrial proteins. Finally, our findings suggest that other insertases which possess a hydrophilic path across the membrane like MTCH2, can also function as scramblases.

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PubMed ID: 38377988

Author Identifiers:

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Record 20 of 274

Title: Winners vs. losers: Schistosoma mansoni intestinal and liver eggs exhibit striking differences in gene expression and immunogenicity

Author(s): Peterková, K (Peterkova, Kristyna); Konecny, L (Konecny, Lukas); Machácek, T (Machacek, Tomas); Jedlicková, L (Jedlickova, Lucie); Winkelmann, F (Winkelmann, Franziska); Sombetzki, M (Sombetzki, Martina); Dvorák, J (Dvorak, Jan)

Source: PLOS PATHOGENS **Volume:** 20 **Issue:** 5 **Article Number:** e1012268 **DOI:** 10.1371/journal.ppat.1012268 **Published Date:** 2024 MAY

Abstract: The eggs of the blood fluke Schistosoma mansoni are the main cause of the clinical manifestations of chronic schistosomiasis. After laying, the egg "winners" attach to the endothelium of the mesenteric vein and, after a period of development, induce the growth of a small granuloma, which facilitates their passage to the intestinal lumen. Egg "losers" carried by the bloodstream to non-specific tissues also undergo full development and induce large granuloma formation, but their life ends there. Although these trapped eggs represent a dead end in the parasite life cycle, the vast majority of studies attempting to describe the biology of the S. mansoni eggs have studied these liver-trapped "losers" instead of migrating intestinal "winners". This raises the fundamental question of how these eggs differ. With robust comparative transcriptomic analysis performed on S. mansoni eggs isolated 7 weeks post infection, we show that gene expression is critically dependent on tissue localization, both in the early and late stages of development. While mitochondrial genes and venom allergen-like proteins are significantly upregulated in mature intestinal eggs, well-described egg immunomodulators IPSE/alpha-1 and omega-1, together with micro-exon genes, are predominantly expressed in liver eggs. In addition, several proteases and protease inhibitors previously implicated in egg-host interactions display clear tissue-specific gene expression patterns. These major differences in gene expression could be then reflected in the observed different ability of liver and intestinal soluble egg antigens to elicit host immune responses and in the shorter viability of miracidia hatched from liver eggs. Our comparative analysis provides a new perspective on the biology of parasite's eggs in the context of their development and tissue localization. These findings could contribute to a broader and more accurate understanding of parasite eggs interactions with the host, which have historically been often restricted to liver eggs and sometimes inaccurately generalized.

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PubMed ID: 38814989

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ISSN: 1553-7366

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Record 21 of 274

Title: The influence of laser focusing conditions on the direct laser acceleration of electrons

Author(s): Tang, H (Tang, H.); Tangtartharakul, K (Tangtartharakul, K.); Babjak, R (Babjak, R.); Yeh, IL (Yeh, I-l); Albert, F (Albert, F.); Chen, H (Chen, H.); Campbell, PT (Campbell, P. T.); Ma, Y (Ma, Y.); Nilson, PM (Nilson, P. M.); Russell, BK (Russell, B. K.); Shaw, JL (Shaw, J. L.); Thomas, AGR (Thomas, A. G. R.); Vranic, M (Vranic, M.); Arefiev, A (Arefiev, A., V); Willingale, L (Willingale, L.)

Source: NEW JOURNAL OF PHYSICS **Volume:** 26 **Issue:** 5 **Article Number:** 053010 **DOI:** 10.1088/1367-2630/ad3be4 **Published Date:** 2024 MAY 1

Abstract: Direct laser acceleration of electrons during a high-energy, picosecond laser interaction with an underdense plasma has been demonstrated to be substantially enhanced by controlling the laser focusing geometry. Experiments using the OMEGA EP facility measured electrons accelerated to maximum energies exceeding 120 times the ponderomotive energy under certain laser focusing, pulse energy, and plasma density conditions. Two-dimensional particle-in-cell simulations show that the laser focusing conditions alter the laser field evolution, channel fields generation, and electron oscillation, all of which contribute to the final electron energies. The optimal laser focusing condition occurs when the transverse oscillation amplitude of the accelerated electron in the channel fields matches the laser beam width, resulting in efficient energy gain. Through this observation, a simple model was developed to calculate the optimal laser focal spot size in more general conditions and is validated by experimental data.

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ISSN: 1367-2630

Record 22 of 274

Title: Synthetically-primed adaptation of Pseudomonas putida to a non-native substrate D-xylose

Author(s): Dvorák, P (Dvorak, Pavel); Burysková, B (Buryskova, Barbora); Popelárova, B (Popelarova, Barbora); Ebert, BE (Ebert, Birgitta E.); Botka, T (Botka, Tibor); Bujdos, D (Bujdos, Dalimil); Sanchez-Pascuala, A (Sanchez-Pascuala, Alberto); Schöttler, H (Schoettler, Hannah); Hayen, H (Hayen, Heiko); de Lorenzo, V (de Lorenzo, Victor); Blank, LM (Blank, Lars M.); Benesik, M (Benesik, Martin)

Source: NATURE COMMUNICATIONS **Volume:** 15 **Issue:** 1 **Article Number:** 2666 **DOI:** 10.1038/s41467-024-46812-9 **Published Date:** 2024 MAR 26

Abstract: To broaden the substrate scope of microbial cell factories towards renewable substrates, rational genetic interventions are often combined with adaptive laboratory evolution (ALE). However, comprehensive studies enabling a holistic understanding of adaptation processes primed by rational metabolic engineering remain scarce. The industrial workhorse Pseudomonas putida was engineered to utilize the non-native sugar D-xylose, but its assimilation into the bacterial biochemical network via the exogenous xylose isomerase pathway remained unresolved. Here, we elucidate the xylose metabolism and establish a foundation for further engineering followed by ALE. First, native glycolysis is derepressed by deleting the local transcriptional regulator gene hexR. We then enhance the pentose phosphate pathway by implanting exogenous transketolase and transaldolase into two lag-shortened strains and allow ALE to finetune the rewired metabolism. Subsequent multilevel analysis and reverse engineering provide detailed insights into the parallel paths of bacterial adaptation to the non-native carbon source, highlighting the enhanced expression of transaldolase and xylose isomerase along with derepressed glycolysis as key events during the process.

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PubMed ID: 38531855

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Record 23 of 274

Title: Hidden Symmetry in Interacting-Quantum-Dot-Based Multiterminal Josephson Junctions

Author(s): Zalom, P (Zalom, Peter); Zonda, M (Zonda, M.); Novotny, T (Novotny, T.)

Source: PHYSICAL REVIEW LETTERS **Volume:** 132 **Issue:** 12 **Article Number:** 126505 **DOI:** 10.1103/PhysRevLett.132.126505 **Published Date:** 2024 MAR 21

Abstract: We study a multiterminal Josephson junction based on an interacting quantum dot coupled to n superconducting BCS leads. Using an Anderson type model of a local level with an arbitrary on-site Coulomb repulsion, we uncover its surprising equivalence with an effective two-terminal junction with

symmetric couplings to appropriately phase-biased leads. Regardless of the strength of the Coulomb interaction, this hidden symmetry enables us to apply well-established numerical and theoretical tools for exact evaluation of various physical quantities, and imposes strict relations among them. Focusing on threeterminal devices, we then demonstrate several phenomena such as the existence of the finite energy band crossings and superconducting transistor and diode effects, as well as current phase relation modulation.

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PubMed ID: 38579211

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Novotny, Tomas	C-7392-2009	0000-0001-7014-4155

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Record 24 of 274

Title: LOFAR detection of extended emission around a mini halo in the galaxy cluster Abell 1413

Author(s): Lusetti, G (Lusetti, G.); Bonafede, A (Bonafede, A.); Lovisari, L (Lovisari, L.); Gitti, M (Gitti, M.); Ettori, S (Ettori, S.); Cassano, R (Cassano, R.); Riseley, CJ (Riseley, C. J.); Govoni, F (Govoni, F.); Brüggen, M (Brueggen, M.); Bruno, L (Bruno, L.); van Weeren, RJ (van Weeren, R. J.); Botteon, A (Botteon, A.); Hoang, DN (Hoang, D. N.); Gastaldello, F (Gastaldello, F.); Ignesti, A (Ignesti, A.); Rossetti, M (Rossetti, M.); Shimwell, TW (Shimwell, T. W.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 683 **Article Number:** A132 **DOI:** 10.1051/0004-6361/202347635 **Published Date:** 2024 MAR 13

Abstract: Context. The relation between giant radio halos and mini halos in galaxy clusters is not understood. The former are usually associated with merging clusters, while the latter are found in relaxed systems. In recent years, the advent of low-frequency radio observations has challenged this dichotomy by finding intermediate objects with a hybrid radio morphology. Aims. We aim to investigate the presence of diffuse radio emission in the cluster Abell 1413 and determine its dynamical status to explore the relation between mini halos and giant radio halos. Methods. We used LOFAR observations centred at 144 MHz to study the diffuse radio emission. To investigate the dynamical state of the system, we used newly analysed XMM-Newton archival data. Abell 1413 shows features that are typically present in both relaxed (e.g., peaked X-ray surface brightness distribution and some large-scale inhomogeneities) and disturbed (e.g., flatter temperature and metallicity profiles) clusters. Results. This suggests that Abell 1413 is neither disturbed nor fully relaxed, and we argue that it is an intermediate-phase cluster. At 144 MHz, we discover a wider diffuse component surrounding the previously known mini halo at the cluster center. By fitting the radio surface-brightness profile with a double-exponential model, we can disentangle the two components. We find an inner mini halo with an e-folding radius, r(e, 1) = 28 +/- 5 kpc, and an extended component with r(e, 2) = 290 +/- 60 kpc. We also evaluated the point-to-point correlation between the radio and X-ray surface brightness, finding a sublinear relation for the outer emission and a superlinear relation for the mini halo. The mini halo and the diffuse emission extend over different scales and show different features, confirming the double nature of the radio emission and suggesting that the mechanisms responsible for the re-acceleration of the radio-emitting particle might be different.

Accession Number: WOS:001184569900004

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Record 25 of 274

Title: Competing Intermolecular and Molecule-Surface Interactions: Dipole-Dipole-Driven Patterns in Mixed Carborane Self-Assembled Monolayers

Author(s): White, KE (White, Katherine E.); Avery, EM (Avery, Erin M.); Cummings, E (Cummings, Edison); Hong, ZX (Hong, Zixiang); Langecker, J (Langecker, Jens); Vetushka, A (Vetushka, Aliaksei); Dusek, M (Dusek, Michal); Machacek, J (Machacek, Jan); Visnak, J (Visnak, Jakub); Endres, J (Endres, Jan); Bastl, Z (Bastl, Zdenek); Mete, E (Mete, Ersen); Alexandrova, AN (Alexandrova, Anastassia N.); Base, T (Base, Tomas); Weiss, PS (Weiss, Paul S.)

Source: CHEMISTRY OF MATERIALS **Volume:** 36 **Issue:** 4 **Pages:** 2085-2095 **DOI:** 10.1021/acs.chemmater.3c03210 **Early Access Date:** FEB 2024 **Published Date:** 2024 FEB 8

Abstract: Carboranedithiol isomers adsorbing with opposite orientations of their dipoles on surfaces are self-assembled together to form mixed monolayers where both lateral dipole-dipole and lateral thiol-thiolate (S-H<middle dot><middle dot><middle dot>S) interactions provide enhanced stability over single-component monolayers. We demonstrate the first instance of the ability to map individual isomers in a mixed monolayer using the model system carboranedithiols on Au{111}. The addition of methyl groups to one isomer provides both an enhanced dipole moment and extra apparent height for differentiation via scanning tunneling microscopy (STM). Associated computational investigations rationalize favorable interactions of mixed pairs and the associated stability changes that arise from these interactions. Both STM images and Monte Carlo simulations yield similarly structured mixed monolayers, where approximately 10% of the molecules have reversed dipole moment orientations but no direct chemical attachment to the surface, leading to homogeneous monolayers with no apparent phase separation. Deprotonating the thiols by depositing the molecules under basic conditions eliminates the lateral S-H<middle dot><middle dot><middle dot>S interactions while accentuating the dipole-dipole forces. The molecular system investigated is composed of isomeric molecules with opposite orientations of dipoles and identical surface packing, which enables the mapping of individual molecules within the mixed monolayers and enables analyses of the contributions of the relatively weak lateral interactions to the overall stability of the assemblies.

Accession Number: WOS:001166534100001

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ISSN: 0897-4756

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Record 26 of 274

Title: Electronic Structure of Metalloporphenes, Antiaromatic Analogues of Graphene

Author(s): Pavlak, I (Pavlak, Ivan); Matasovic, L (Matasovic, Lujo); Buchanan, EA (Buchanan, Eric A.); Michl, J (Michl, Josef); Roncevic, I (Roncevic, Igor)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 146 **Issue:** 6 **Pages:** 3992-4000 **DOI:** 10.1021/jacs.3c12079 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN 31

Abstract: Zinc porphene is a two-dimensional material made of fully fused zinc porphyrins in a tetragonal lattice. It has a fully conjugated pi-system, making it similar to graphene. Zinc porphene has recently been synthesized, and a combination of rough conductivity measurements and infrared and Raman spectroscopies all suggested that it is a semiconductor (Magnera, T.F. et al. Porphene and Porphite as Porphyrin Analogs of Graphene and Graphite, Nat. Commun. 2023, 14, 6308). This is in contrast with all previous predictions of its electronic structure, which indicated metallic conductivity. We show that the gap-opening in zinc porphene is caused by a Peierls distortion of its unit cell from square to rectangular, thus giving the first account of its electronic structure in agreement with the experiment. Accounting for this distortion requires proper treatment of electron delocalization, which can be done using hybrid functionals with a substantial amount of exact exchange. Such a functional, PBE38, is then applied to predict the properties of many first transition row metalloporphenes, some of which have already been prepared. We find that changing the metal strongly affects the electronic structure of metalloporphenes, resulting in a rich variety of both metallic conductors and semiconductors, which may be of great interest to molecular electronics and spintronics. Properties of these materials are mostly governed by the extent of the Peierls distortion and the number of electrons in their pi-system, analogous to changes in aromaticity observed in cyclic conjugated molecules upon oxidation or reduction. These results give an account of how the concept of antiaromaticity can be extended to periodic systems.

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PubMed ID: 38294407

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ISSN: 0002-7863

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Record 27 of 274

Title: A comparative study of cross-lingual sentiment analysis

Author(s): Pribán, P (Priban, Pavel); Smíd, J (Smid, Jakub); Steinberger, J (Steinberger, Josef); Mistera, A (Mistera, Adam)

Source: EXPERT SYSTEMS WITH APPLICATIONS **Volume:** 247 **Article Number:** 123247 **DOI:** 10.1016/j.eswa.2024.123247 **Early Access Date:** JAN 2024 **Published Date:** 2024 AUG 1

Abstract: This paper presents a detailed comparative study of the zero -shot cross -lingual sentiment analysis. Namely, we use modern multilingual Transformer -based models and linear transformations combined with CNN and LSTM neural networks. We evaluate their performance in Czech, French, and English. We aim to compare and assess the models' ability to transfer knowledge across languages and discuss the trade-off between their performance and training/inference speed. We build strong monolingual baselines comparable with the current SotA approaches, achieving state-of-the-art results in Czech (96.0% accuracy) and French (97.6% accuracy). Next, we compare our results with the latest large language models (LLMs), i.e., Llama 2 and ChatGPT. We show that the large multilingual Transformer -based XLM-R model consistently outperforms all other cross -lingual approaches in zero -shot cross -lingual sentiment classification, surpassing them by at least 3%. Next, we show that the smaller

Transformer -based models are comparable in performance to older but much faster methods with linear transformations. The best -performing model with linear transformation achieved an accuracy of 92.1% on the French dataset, compared to 90.3% received by the smaller XLM-R model. Notably, this performance is achieved with just approximately 0.01 of the training time required for the XLM-R model. It underscores the potential of linear transformations as a pragmatic alternative to resource -intensive and slower Transformer -based models in real -world applications. The LLMs achieved impressive results that are on par or better, at least by 1%-3%, but with additional hardware requirements and limitations. Overall, this study contributes to understanding cross -lingual sentiment analysis and provides valuable insights into the strengths and limitations of cross -lingual approaches for sentiment analysis.

Accession Number: WOS:001171252000001

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Record 28 of 274

Title: How the Support Defines Properties of 2D Metal-Organic Frameworks: Fe-TCNQ on Graphene versus Au(111)

Author(s): Jakub, Z (Jakub, Zdenek); Shahsavar, A (Shahsavar, Azin); Planer, J (Planer, Jakub); Hruza, D (Hruza, Dominik); Herich, O (Herich, Ondrej); Procházka, P (Prochazka, Pavel); Cechal, J (Cechal, Jan)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 146 **Issue:** 5 **Pages:** 3471-3482 **DOI:** 10.1021/jacs.3c13212 **Published Date:** 2024 JAN 22

Abstract: The functionality of 2D metal-organic frameworks (MOFs) is crucially dependent on the local environment of the embedded metal atoms. These atomic-scale details are best ascertained on MOFs supported on well-defined surfaces, but the interaction with the support often changes the MOF properties. We elucidate the extent of this effect by comparing the Fe-TCNQ 2D MOF on two weakly interacting supports: graphene and Au(111). We show that the Fe-TCNQ on graphene is nonplanar with iron in quasi-tetrahedral sites, but on Au(111) it is planarized by stronger van der Waals interaction. The differences in physical and electronic structures result in distinct properties of the supported 2D MOFs. The d (2)(z)center position is shifted by 1.4 eV between Fe sites on the two supports, and dramatic differences in chemical reactivity are experimentally identified using a TCNQ probe molecule. These results outline the limitations of common on-surface approaches using metal supports and show that the intrinsic MOF properties can be partially retained on graphene.

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PubMed ID: 38253402

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Record 29 of 274

Title: Rapid diversification of a free-living protist is driven by adaptation to climate and habitat

Author(s): Skaloud, P (Skaloud, Pavel); Jadrná, I (Jadrna, Iva); Dvorák, P (Dvorak, Petr); Skvorová, Z (Skvorova, Zuzana); Pusztai, M (Pusztai, Martin); Certnerová, D (Certnerova, Dora); Bestová, H (Bestova, Helena); Rengefors, K (Rengefors, Karin)

Source: CURRENT BIOLOGY **Volume:** 34 **Issue:** 1 **DOI:** 10.1016/j.cub.2023.11.046 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN 8

Abstract: Microbial eukaryotes (protists) have major functional roles in aquatic ecosystems, including the biogeochemical cycling of elements as well as occupying various roles in the food web. Despite their importance for ecosystem function, the factors that drive diversification in protists are not known. Here, we aimed to identify the factors that drive differentiation and, subsequently, speciation in a free-living protist, Synura petersenii (Chrysophyceae). We sampled five different geographic areas and utilized population genomics and quantitative trait analyses. Habitat and climate were the major drivers of diversification on the local geographical scale, while geography played a role over longer distances. In addition to conductivity and temperature, precipitation was one of the most important environmental drivers of differentiation. Our results imply that flushing episodes (floods) drive microalgal adaptation to different niches, highlighting the potential for rapid diversification in protists.

Accession Number: WOS:001154618200001

PubMed ID: 38103550

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Rengefors, Karin	K-5873-2019	
Skaloud, Pavel	F-3103-2011	

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Record 30 of 274

Title: Synthesis and broad-spectrum biocidal effect of novel gemini quaternary ammonium compounds

Author(s): Zivna, N (Zivna, Natalie); Hympanova, M (Hympanova, Michaela); Dolezal, R (Dolezal, Rafael); Markova, A (Markova, Aneta); Pulkrabkova, L (Pulkrabkova, Lenka); Strakova, H (Strakova, Hana); Sleha, R (Sleha, Radek); Prchal, L (Prchal, Lukas); Brozkova, I (Brozkova, Iveta); Motkova, P (Motkova, Petra); Sefrankova, L (Sefrankova, Laura); Soukup, O (Soukup, Ondrej); Marek, J (Marek, Jan)

Source: BIOORGANIC CHEMISTRY **Volume:** 151 **Article Number:** 107646 **DOI:** 10.1016/j.bioorg.2024.107646 **Early Access Date:** JUL 2024 **Published Date:** 2024 OCT

Abstract: Since the discovery of antimicrobial agents, the misuse of antibiotics has led to the emergence of bacterial strains resistant to both antibiotics and common disinfectants like quaternary ammonium compounds (QACs). A new class, 'gemini' QACs, which contain two polar heads, has shown promise. Octenidine (OCT), a representative of this group, is effective against resistant microorganisms but has limitations such as low solubility and high cytotoxicity. In this study, we developed 16 novel OCT derivatives. These compounds were subjected to in silico screening to predict their membrane permeation. Testing against nosocomial bacterial strains (G+ and G-) and their biofilms revealed that

most compounds were highly effective against G+ bacteria, while compounds 7, 8, and 10-12 were effective against G-bacteria. Notably, compounds 6-8 were significantly more effective than OCT and BAC standards across the bacterial panel. Compound 12 stood out due to its low cytotoxicity and broadspectrum antimicrobial activity, comparable to OCT. It also demonstrated impressive antifungal activity. Compound 1 was highly selective to fungi and four times more effective than OCT without its cytotoxicity. Several compounds, including 4, 6, 8, 9, 10, and 12, showed strong virucidal activity against murine cytomegalovirus and herpes simplex virus 1. In conclusion, these gemini QACs, especially compound 12, offer a promising alternative to current disinfectants, addressing emerging resistances with their enhanced antimicrobial, antifungal, and virucidal properties.

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PubMed ID: 39032408

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Record 31 of 274

Title: CoVAMPnet: Comparative Markov State Analysis for Studying Effects of Drug Candidates on Disordered Biomolecules

Author(s): Marques, S (Marques, SergioM.); Kouba, P (Kouba, Petr); Legrand, A (Legrand, Anthony); Sedlar, J (Sedlar, Jiri); Disson, L (Disson, Lucas); Planas-Iglesias, J (Planas-Iglesias, Joan); Sanusi, Z (Sanusi, Zainab); Kunka, A (Kunka, Antonin); Damborsky, J (Damborsky, Jiri); Pajdla, T (Pajdla, Tomas); Prokop, Z (Prokop, Zbynek); Mazurenko, S (Mazurenko, Stanislav); Sivic, J (Sivic, Josef); Bednar, D (Bednar, David)

Source: JACS AU **Volume:** 4 **Issue:** 6 **Pages:** 2228-2245 **DOI:** 10.1021/jacsau.4c00182 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 28

Abstract: Computational study of the effect of drug candidates on intrinsically disordered biomolecules is challenging due to their vast and complex conformational space. Here, we developed a comparative Markov state analysis (CoVAMPnet) framework to quantify changes in the conformational distribution and dynamics of a disordered biomolecule in the presence and absence of small organic drug candidate molecules. First, molecular dynamics trajectories are generated using enhanced sampling, in the presence and absence of small molecule drug candidates, and ensembles of soft Markov state models (MSMs) are learned for each system using unsupervised machine learning. Second, these ensembles of learned MSMs are aligned across different systems based on a solution to an optimal transport problem. Third, the directional importance of inter-residue distances for the assignment to different conformational states is assessed by a discriminative analysis of aggregated neural network gradients. This final step provides interpretability and biophysical context to the learned MSMs. We applied this novel computational framework to assess the effects of ongoing phase 3 therapeutics tramiprosate (TMP) and its metabolite 3-sulfopropanoic acid (SPA) on the disordered A beta 42 peptide involved in Alzheimer's disease. Based on adaptive sampling molecular dynamics and CoVAMPnet analysis, we observed that both TMP and SPA preserved more structured conformations of A beta 42 by interacting nonspecifically with charged residues. SPA impacted A beta 42 more than TMP, protecting alpha-helices and suppressing the formation of aggregation-prone beta-strands. Experimental biophysical analyses showed only mild effects of TMP/SPA on A beta 42 and activity enhancement by the endogenous metabolization of TMP

into SPA. Our data suggest that TMP/SPA may also target biomolecules other than A beta peptides. The CoVAMPnet method is broadly applicable to study the effects of drug candidates on the conformational behavior of intrinsically disordered biomolecules.

Accession Number: WOS:001234423200001

PubMed ID: 38938816

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eISSN: 2691-3704

Record 32 of 274

Title: HIV-1 Infection Reduces NAD Capping of Host Cell snRNA and snoRNA

Author(s): Benoni, B (Benoni, Barbora); Potuzník, JF (Potuznik, Jiri Frantiscek); Skríba, A (Skriba, Anton); Benoni, R (Benoni, Roberto); Trylcova, J (Trylcova, Jana); Tulpa, M (Tulpa, Matous); Spustová, K (Spustova, Kristina); Grab, K (Grab, Katarzyna); Mititelu, MB (Mititelu, Maria-Bianca); Paces, J (Paces, Jan); Weber, J (Weber, Jan); Stanek, D (Stanek, David); Kowalska, J (Kowalska, Joanna); Bednarova, L (Bednarova, Lucie); Keckesova, Z (Keckesova, Zuzana); Vopalensky, P (Vopalensky, Pavel); Gahurova, L (Gahurova, Lenka); Cahova, H (Cahova, Hana)

Source: ACS CHEMICAL BIOLOGY **Volume:** 19 **Issue:** 6 **Pages:** 1243-1249 **DOI:** 10.1021/acschembio.4c00151 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 15

Abstract: Nicotinamide adenine dinucleotide (NAD) is a critical component of the cellular metabolism and also serves as an alternative 5 ' cap on various RNAs. However, the function of the NAD RNA cap is still under investigation. We studied NAD capping of RNAs in HIV-1-infected cells because HIV-1 is responsible for the depletion of the NAD/NADH cellular pool and causing intracellular pellagra. By applying the NAD captureSeq protocol to HIV-1-infected and uninfected cells, we revealed that four snRNAs (e.g., U1) and four snoRNAs lost their NAD cap when infected with HIV-1. Here, we provide evidence that the presence of the NAD cap decreases the stability of the U1/HIV-1 pre-mRNA duplex. Additionally, we demonstrate that reducing the quantity of NAD-capped RNA by overexpressing the NAD RNA decapping enzyme DXO results in an increase in HIV-1 infectivity. This suggests that NAD capping is unfavorable for HIV-1 and plays a role in its infectivity.

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PubMed ID: 38747804

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ISSN: 1554-8929

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Record 33 of 274

Title: 2D nature of magnetic states at SnO₂ surfaces: a combined experimental and theoretical study

Author(s): Hong, NH (Hong, Nguyen Hoa); Friák, M (Friak, Martin); Pazourek, P (Pazourek, Petr); Pham, NS (Pham, Nguyen Sy); Nhu, TQ (Nhu, Tran Quynh); Kiaba, M (Kiaba, Michal); Gazdová, K (Gazdova, Kristyna); Pavlu, J (Pavlu, Jana)

Source: RSC ADVANCES **Volume:** 14 **Issue:** 19 **Pages:** 13583-13590 **DOI:** 10.1039/d4ra00734d **Published Date:** 2024 APR 22

Abstract: For undoped SnO2, room temperature ferromagnetism could be seen uniquely in 2-dimensional configurations, particularly in ultra-thin films (whose thickness is ideally below 100 nm). Both bulk samples and nano-powders of pristine SnO2 are diamagnetic, indicating that a 2D surface is a key point in shaping up the magnetic properties in SnO2. As a complement to our experiments, we have performed a series of quantum-mechanical calculations for the bulk rutile-structure SnO2 as well as its (001) and (101) surfaces. The calculations included several atomic configurations with and without vacancies in/under the studied surfaces. The stability of the non-magnetic ground state of rutile SnO2 bulk was cross-checked and confirmed by its phonon spectrum computed within the harmonic approximation. Regarding the surfaces, the bulk-like (001) surface containing Sn vacancies has turned out to be ferromagnetic, while the shift of Sn vacancies under the surface resulted in a more complex ferrimagnetic state. The bulk-like (001) surface without vacancies and that with the O vacancies are predicted to be non-magnetic. Regarding the (101) surfaces, those terminated by a single layer of oxygen atoms and those terminated by tin atoms are non-magnetic, while a surface terminated by two layers of oxygen has turned out to be ferromagnetic.

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PubMed ID: 38665488

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Friak, Martin	IAN-4977-2023	0000-0003-1892-6859
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eISSN: 2046-2069

Record 34 of 274

Title: Post-dynamical inspiral phase of common envelope evolution The role of magnetic fields

Author(s): Gagnier, D (Gagnier, Damien); Pejcha, O (Pejcha, Ondrej)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 683 **Article Number:** A4 **DOI:** 10.1051/0004-6361/202348383 **Published Date:** 2024 FEB 28

Abstract: During common envelope evolution, an initially weak magnetic field may undergo amplification by interacting with spiral density waves and turbulence generated in the stellar envelope by the inspiralling companion. Using 3D magnetohydrodynamical simulations on adaptively refined spherical grids with excised central regions, we studied the amplification of magnetic fields and their effect on the envelope structure, dynamics, and the orbital evolution of the binary during the post-dynamical inspiral phase. About 95% of magnetic energy amplification arises from magnetic field stretching, folding, and winding due to differential rotation and turbulence while compression against magnetic pressure accounts for the remaining similar to 5%. Magnetic energy production peaks at a scale of 3ab, where ab is the semimajor axis of the central binary's orbit. Because the magnetic energy

production declines at large radial scales, the conditions are not favorable for the formation of magnetically collimated bipolar jet-like outflows unless they are generated on small scales near the individual cores, which we did not resolve. Magnetic fields have a negligible impact on binary orbit evolution, mean kinetic energy, and the disk-like morphology of angular momentum transport, but turbulent Maxwell stress can dominate Reynolds stress when accretion onto the central binary is allowed, leading to an alpha-disk parameter of similar or equal to 0.034. Finally, we discovered accretion streams arising from the stabilizing effect of the magnetic tension from the toroidal field about the orbital plane, which prevents overdensities from being destroyed by turbulence and enables them to accumulate mass and eventually migrate toward the binary.

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Record 35 of 274

Title: Discovering Electrochemistry with an Electrochemistry-Informed Neural Network (ECINN)

Author(s): Chen, HT (Chen, Haotian); Yang, MJ (Yang, Minjun); Smetana, B (Smetana, Bedrich); Novak, V (Novak, Vlastimil); Matejka, V (Matejka, Vlastimil); Compton, RG (Compton, Richard G.)

Source: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 63 **Issue:** 13 **DOI:** 10.1002/anie.202315937 **Early Access Date:** FEB 2024 **Published Date:** 2024 MAR 22

Abstract: Machine learning is increasingly integrated into chemistry research by guiding experimental procedures, correlating structure and function, interpreting large experimental datasets, to distill scientific insights that might be challenging with traditional methods. Such applications, however, largely focus on gaining insights via big data and/or big computation, while neglecting the valuable chemical prior knowledge dwelling in chemists' minds. In this paper, we introduce an Electrochemistry-Informed Neural Network (ECINN) by explicitly embedding electrochemistry priors including the Butler-Volmer (BV), Nernst and diffusion equations on the backbone of neural networks for multi-task discovery of electrochemistry parameters. We applied the ECINN to voltammetry experiments of Fe2+/Fe3+ ${{\rm F}{{\rm e}}<^>{2+}/{\rm F}{{\rm e}}<^>{3+}}$ and RuNH362+/RuNH363+ ${{\rm R}{\rm u}{\left({\rm N}{{\rm H}}_{3}\right)}_{6}<^>{2+{\rm \ }}/{\rm R}{\rm u}{\left({\rm N}{{\rm H}}_{3}\right)}_{6}<^>{3+{\rm \ }}}$ redox couples to discover electrode kinetics and mass transport parameters. Notably, ECINN seamlessly integrated mass transport with BV to analyze the entire voltammogram to infer transfer coefficients directly, so offering a new approach to Tafel analysis by outdating various mass transport correction methods. In addition, ECINN can help discover the nature of electron transfer and is shown to refute incorrect physics if imposed. This work encourages chemists to embed their domain knowledge into machine learning models to start a new paradigm of chemistry-informed machine learning for better accountability, interpretability, and generalization. Electrochemistry-Informed Neural Network (ECINN) embeds chemistry prior knowledge including the Bulter-Volmer, Nernst and Diffusion equation to discover electrode kinetics and mass transport parameter simultaneously from sparse experiments. ECINN seamlessly integrates mass transport and BV equation and provides arguably the best Tafel analysis method. This work encourages embedding domain knowledge to realize strong intelligence with sparse data.+ image

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ISSN: 1433-7851

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Record 36 of 274

Title: Exploring the radio loudness of SDSS quasars with spectral stacking

Author(s): Arnaudova, MI (Arnaudova, M., I); Smith, DJB (Smith, D. J. B.); Hardcastle, MJ (Hardcastle, M. J.); Das, S (Das, S.); Drake, A (Drake, A.); Duncan, K (Duncan, K.); Guerkan, G (Guerkan, G.); Magliocchetti, M (Magliocchetti, M.); Morabito, LK (Morabito, L. K.); Petley, JW (Petley, J. W.); Shenoy, S (Shenoy, S.); Tasse, C (Tasse, C.)

Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY **Volume:** 528 **Issue:** 3 **Pages:** 4547-4567 **DOI:** 10.1093/mnras/stae233 **Early Access Date:** FEB 2024 **Published Date:** 2024 FEB 7

Abstract: We use new 144 MHz observations over 5634 deg(2) from the LOFAR (Low Frequency Array) Two-metre Sky Survey (LoTSS) to compile the largest sample of uniformly selected, spectroscopically confirmed quasars from the 14th data release of the Sloan Digital Sky Survey (SDSS-DR14). Using the classical definition of radio loudness, R = log (L-1.4GHz/L-i), we identify 3697 radio-loud (RL) and 111 132 radio-quiet (RQ) sources at $0.6 < z < 3.4$. To study their properties, we develop a new rest-frame spectral stacking algorithm, designed with forthcoming massively multiplexed spectroscopic surveys in mind, and use it to create high signal-to-noise composite spectra of each class, matched in redshift and absolute i-band magnitude. We show that RL quasars have redder continuum and enhanced [O II] emission than their RQ counterparts. These results persist when additionally matching in black hole mass, suggesting that this parameter is not the defining factor in making a quasi-stellar object (QSO) RL. We find that these features are not gradually varying as a function of radio loudness, but are maintained even when probing deeper into the RQ population, indicating that a clear-cut division in radio loudness is not apparent. Upon examining the star formation rates (SFRs) inferred from the [O II] emission line, with the contribution from active galactic nucleus removed using the [Ne V] line, we find that RL quasars have a significant excess of star formation relative to RQ quasars out to $z = 1.9$ at least. Given our findings, we suggest that RL sources either preferably reside in gas-rich systems with rapidly spinning black holes, or represent an earlier obscured phase of QSO evolution.

Accession Number: WOS:001159352200012

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ISSN: 0035-8711

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Record 37 of 274

Title: Acceleration of Molecular Simulations by Parametric Time-Lagged tSNE Metadynamics

Author(s): Hradiská, H (Hradiska, Helena); Kurecka, M (Kurecka, Martin); Beránek, J (Beranek, Jan); Tedeschi, G (Tedeschi, Guglielmo); Visnovsky, V (Visnovsky, Vladimir); Krenek, A (Krenek, Ales);

Spiwok, V (Spiwok, Vojtech)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 128 **Issue:** 4 **Pages:** 903-913 **DOI:** 10.1021/acs.jpcb.3c05669 **Published Date:** 2024 JAN 18

Abstract: The potential of molecular simulations is limited by their computational costs. There is often a need to accelerate simulations using some of the enhanced sampling methods. Metadynamics applies a history-dependent bias potential that disfavors previously visited states. To apply metadynamics, it is necessary to select a few properties of the system-collective variables (CVs) that can be used to define the bias potential. Over the past few years, there have been emerging opportunities for machine learning and, in particular, artificial neural networks within this domain. In this broad context, a specific unsupervised machine learning method was utilized, namely, parametric time-lagged t-distributed stochastic neighbor embedding (ptltSNE) to design CVs. The approach was tested on a Trp-cage trajectory (tryptophan cage) from the literature. The trajectory was used to generate a map of conformations, distinguish fast conformational changes from slow ones, and design CVs. Then, metadynamic simulations were performed. To accelerate the formation of the alpha-helix, we added the alpha-RMSD collective variable. This simulation led to one folding event in a 350 ns metadynamics simulation. To accelerate degrees of freedom not addressed by CVs, we performed parallel tempering metadynamics. This simulation led to 10 folding events in a 200 ns simulation with 32 replicas.

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PubMed ID: 38237064

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ISSN: 1520-6106

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Record 38 of 274

Title: Exploring the Role of Globular Domain Locations on an Intrinsically Disordered Region of p53: A Molecular Dynamics Investigation

Author(s): Bakker, MJ (Bakker, Michael J.); Sorensen, HV (Sorensen, Henrik V.); Skepö, M (Skepo, Marie)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 20 **Issue:** 3 **Pages:** 1423-1433 **DOI:** 10.1021/acs.jctc.3c00971 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN 17

Abstract: The pre-tetramerization loop (PTL) of the human tumor suppressor protein p53 is an intrinsically disordered region (IDR) necessary for the tetramerization process, and its flexibility contributes to the essential conformational changes needed. Although the IDR can be accurately simulated in the traditional manner of molecular dynamics (MD) with the end-to-end distance (EEdist) unhindered, we sought to explore the effects of restraining the EEdist to the values predicted by electron microscopy (EM) and other distances. Simulating the PTL trajectory with a restrained EEdist , we found an increased agreement of nuclear magnetic resonance (NMR) chemical shifts with experiments. Additionally, we observed a plethora of secondary structures and contacts that only appear when the trajectory is restrained. Our findings expand the understanding of the tetramerization of p53 and provide insight into how mutations could make the protein impotent. In particular, our findings demonstrate the importance of restraining the EEdist in studying IDRs and how their conformations change under different conditions. Our results provide a better understanding of the PTL and the conformational

dynamics of IDRs in general, which are useful for further studies regarding mutations and their effects on the activity of p53.

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PubMed ID: 38230670

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ISSN: 1549-9618

eISSN: 1549-9626

Record 39 of 274

Title: Measuring the energy for the molecular graphs of antiviral agents: Hydroxychloroquine, Chloroquine and Remdesivir

Author(s): Aftab, MH (Aftab, Muhammad Haroon); Akgül, A (Akgul, Ali); Riaz, MB (Riaz, Muhammad Bilal); Hussain, M (Hussain, Muhammad); Jebreen, K (Jebreen, Kamel); Kanj, H (Kanj, Hassan)

Source: SOUTH AFRICAN JOURNAL OF CHEMICAL ENGINEERING **Volume:** 47 **Pages:** 333-337 **DOI:** 10.1016/j.sajce.2023.12.006 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN

Abstract: We consider the energy for the molecular graphs of antiviral agents like Hydroxychloroquine, Remdesivir and Chloroquine. These drugs play a vital role in the treatment of COVID-19. Let Gamma(1), Gamma(2) and Gamma(3) be the n-dimensional graphs of the molecular structures of antiviral agents Hydroxychloroquine, Chloroquine and Remdesivir, respectively. We define their energies as E '(Gamma(1)) = Sigma vertical bar lambda(i)'vertical bar, E '(Gamma 2) = Sigma vertical bar lambda(j)'vertical bar and E '(Gamma 3) = Sigma vertical bar lambda(k)'vertical bar, respectively. Where the sets {lambda(1)'(Gamma(1)), lambda(2)'(Gamma(1)), lambda(3)'(Gamma(1)), ..., lambda(n)'(Gamma(1))}, {lambda(1)'(Gamma(2)), lambda(2)'(Gamma(2)), lambda(3)'(Gamma(2)), ..., lambda(n)'(Gamma(2))} and { lambda(1)'(Gamma 3), lambda(2)'(Gamma 3), lambda(3)'(Gamma 3), ..., lambda(n)'(Gamma 3)} depict the eigenvalues for the adjacency matrices of Gamma 1, Gamma 2 and Gamma 3, respectively. We have developed some basic ideas and properties in order to measure the energies for the antiviral agents Hydroxychloroquine, Chloroquine and Remdesivir.

Accession Number: WOS:001292453700001

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ISSN: 1026-9185

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Record 40 of 274

Title: Sex-biased gene content is associated with sex chromosome turnover in Danaini butterflies

Author(s): Mora, P (Mora, Pablo); Hospodarska, M (Hospodarska, Monika); Volenikova, AC (Volenikova, Anna Chung); Koutecky, P (Koutecky, Petr); Stundlova, J (Stundlova, Jana); Dalikova, M (Dalikova, Martina); Walters, JR (Walters, James R.); Nguyen, P (Nguyen, Petr)

Source: MOLECULAR ECOLOGY **Volume:** 33 **Issue:** 24 **Special Issue:** SI **DOI:** 10.1111/mec.17256 **Early Access Date:** JAN 2024 **Published Date:** 2024 DEC

Abstract: Sex chromosomes play an outsized role in adaptation and speciation, and thus deserve particular attention in evolutionary genomics. In particular, fusions between sex chromosomes and autosomes can produce neo-sex chromosomes, which offer important insights into the evolutionary dynamics of sex chromosomes. Here, we investigate the evolutionary origin of the previously reported Danaus neo-sex chromosome within the tribe Danaini. We assembled and annotated genomes of Tirumala septentrionis (subtribe Danaina), Ideopsis similis (Amaurina), Idea leuconoe (Euploeina) and Lycorea halia (Itunina) and identified their Z-linked scaffolds. We found that the Danaus neo-sex chromosome resulting from the fusion between a Z chromosome and an autosome corresponding to the Melitaea cinxia chromosome (McChr) 21 arose in a common ancestor of Danaina, Amaurina and Euploina. We also identified two additional fusions as the W chromosome further fused with the synteny block McChr31 in I. similis and independent fusion occurred between ancestral Z chromosome and McChr12 in L. halia. We further tested a possible role of sexually antagonistic selection in sex chromosome turnover by analysing the genomic distribution of sex-biased genes in I. leuconoe and L. halia. The autosomes corresponding to McChr21 and McChr31 involved in the fusions are significantly enriched in female- and male-biased genes, respectively, which could have hypothetically facilitated fixation of the neo-sex chromosomes. This suggests a role of sexual antagonism in sex chromosome turnover in Lepidoptera. The neo-Z chromosomes of both I. leuconoe and L. halia appear fully compensated in somatic tissues, but the extent of dosage compensation for the ancestral Z varies across tissues and species.

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PubMed ID: 38180347

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ISSN: 0962-1083

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Record 41 of 274

Title: Computational Fluid Dynamics Calculations of Moderator Heat and Fluid Flow of Small Modular Heavy Water Reactor

Author(s): Korinek, T (Korinek, Tomas); Skoda, R (Skoda, Radek); Lovecky, M (Lovecky, Martin); Burian, O (Burian, Ondrej)

Source: JOURNAL OF NUCLEAR ENGINEERING AND RADIATION SCIENCE **Volume:** 10 **Issue:** 1 **Article Number:** 014501 **DOI:** 10.1115/1.4063007 **Published Date:** 2024 JAN 1

Abstract: The heavy water reactor concept Teplator is a pressure channel type reactor with independent systems for the primary coolant and the moderator. The present study analyses the low-pressure moderator cooling system of Teplator during full-power operation. The moderator is heated from neutron thermalization, gamma rays absorption, fission product decay, and decay of activation products. Additionally, heat transfer from the coolant channels has to be taken in the analyses of the moderator cooling system. Preliminary thermal-hydraulic analyses of the cooling system are supplemented by computational fluid dynamics (CFD) simulations of heat and fluid flow in the moderator's vessel, emphasizing flow-type regimes. Results from CFD simulations showed that the buoyancy-dominated flow (case MF-22) resulted in a higher thermal stratification and high moderator temperature close to the upper plate of the moderator vessel. The inertia-dominated flow regime MF-90 resulted in good mixing of the moderator and a low thermal stratification in the vessel. Finally, the midmass flow rate regime

MF-45 was identified as a transitional region from a buoyancy-dominated to a mix-type regime.

Accession Number: WOS:001133944500007

Author Identifiers:

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ISSN: 2332-8983

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Record 42 of 274

Title: Electronic nonequilibrium effect in ultrafast-laser-irradiated solids

Author(s): Medvedev, N (Medvedev, Nikita)

Source: PHYSICA SCRIPTA **Volume:** 99 **Issue:** 1 **Article Number:** 015934 **DOI:** 10.1088/1402-4896/ad13df **Published Date:** 2024 JAN 1

Abstract: This paper describes the effects of electronic nonequilibrium in a simulation of ultrafast laser irradiation of materials. The simulation scheme based on tight-binding molecular dynamics, in which the electronic populations are traced with a combined Monte Carlo and Boltzmann equation, enables the modeling of nonequilibrium, nonthermal, and nonadiabatic (electron-phonon coupling) effects simultaneously. The electron-electron thermalization is described within the relaxation-time approximation, which automatically restores various known limits such as instantaneous thermalization (the thermalization time tau e-e -> 0) and Born-Oppenheimer (BO) approximation (tau e-e ->infinity). The results of the simulation suggest that the non-equilibrium state of the electronic system slows down electron-phonon coupling with respect to the electronic equilibrium case in all studied materials: metals, semiconductors, and insulators. In semiconductors and insulators, it also alters the damage threshold of ultrafast nonthermal phase transitions induced by modification of the interatomic potential due to electronic excitation. It is demonstrated that the models that exclude electron-electron thermalization (using the assumption of tau e-e ->infinity, such as BO or Ehrenfest approximations) may produce qualitatively different results, and a reliable model should include all three effects: electronic nonequilibrium, nonadiabatic electron-ion coupling, and nonthermal evolution of interatomic potential.

Accession Number: WOS:001128694700001

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ISSN: 0031-8949

eISSN: 1402-4896

Record 43 of 274

Title: Cationic polaron delocalization in porphyrin nanoribbons

Author(s): Kopp, SM (Kopp, Sebastian M.); Deng, JR (Deng, Jie-Ren); Redman, AJ (Redman, Ashley J.); Gotfredsen, H (Gotfredsen, Henrik); Jacobs, RMJ (Jacobs, Robert M. J.); Anderson, HL (Anderson, Harry L.); Timmel, CR (Timmel, Christiane R.)

Source: CHEM **Volume:** 10 **Issue:** 12 **DOI:** 10.1016/j.chempr.2024.07.011 **Early Access Date:** DEC 2024 **Published Date:** 2024 DEC 12

Abstract: Long-range delocalization of unpaired electrons in organic p-conjugated oligomers is an important requirement to achieve high charge carrier mobilities in molecular transistors. We have investigated the polaron de- localization in the radical cations of a series of $,meso,$-edge-fused porphyrin oligomers consisting of up to 18 porphyrin units by a combination of cw-EPR, 1 H, and14N

electron-nuclear double resonance (ENDOR),14N hyperfine sublevel correlation (HYSCORE), and vis-NIR-MIR spectroscopy, supported by density functional theory (DFT) calculations and simulations. The results demonstrate coherent delocalization of the radical cation over more than 10 porphyrin units, which corresponds to an effective coherence length >8.5 nm. We discovered a remarkably non-uniform distribution of the radical spin density and an increase in phase memory time with increasing delocalization length (up to Tm z 4 ms at 50 K). This study opens new avenues toward the design of molecular electronic and spintronic materials.

Accession Number: WOS:001386156400001

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Anderson, Harry	E-7843-2011	
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ISSN: 2451-9294

Record 44 of 274

Title: Satellite monitoring of long period ocean-induced magnetic field variations

Author(s): Finlay, CC (Finlay, Christopher C.); Velímsky, J (Velimsky, Jakub); Kloss, C (Kloss, Clemens); Blangsboll, RM (Blangsboll, Rasmus M.)

Source: PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A-MATHEMATICAL PHYSICAL AND ENGINEERING SCIENCES **Volume:** 382 **Issue:** 2286 **Article Number:** 20240077 **DOI:** 10.1098/rsta.2024.0077 **Published Date:** 2024 DEC 2

Abstract: Satellite magnetic field observations have the potential to provide valuable information on dynamics, heat content and salinity throughout the ocean. Here, we present the expected spatio-temporal characteristics of the ocean-induced magnetic field (OIMF) at satellite altitude on periods of months to decades. We compare these to the characteristics of other sources of Earth's magnetic field, and discuss whether it is feasible for the OIMF to be retrieved and routinely monitored from space. We focus on large length scales (spherical harmonic degrees up to 30) and periods from one month up to 5 years. To characterize the expected ocean signal, we make use of advanced numerical simulations taking high-resolution oceanographic inputs and solve the magnetic induction equation in three dimensions, including galvanic coupling and self-induction effects. We find the time-varying ocean-induced signal dominates over the primary source of the internal field, the core dynamo, at high spherical harmonic degree with the cross-over taking place at degrees 13-19 depending on the considered period. The ionospheric and magnetospheric fields (including their Earth-induced counterparts) have most power on periods shorter than one month and are expected to be mostly zonal in magnetic coordinates at satellite altitude. Based on these findings, we discuss future prospects for isolating and monitoring long period OIMF variations using data collected by present and upcoming magnetic survey satellites.This article is part of the theme issue 'Magnetometric remote sensing of Earth and planetary oceans'.

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PubMed ID: 39617037

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Record 45 of 274

Title: Dynamics of quasi-periodic, bifurcation, sensitivity and three-wave solutions for (n+1)-dimensional generalized Kadomtsev-Petviashvili equation

Author(s): Rafiq, MH (Rafiq, Muhammad Hamza); Riaz, MB (Riaz, Muhammad Bilal); Basendwah, GA (Basendwah, Ghada Ali); Raza, N (Raza, Nauman); Rafiq, MN (Rafiq, Muhammad Naveed)

Source: PLOS ONE **Volume:** 19 **Issue:** 8 **Article Number:** e0305094 **DOI:** 10.1371/journal.pone.0305094 **Published Date:** 2024 AUG 27

Abstract: This study endeavors to examine the dynamics of the generalized Kadomtsev-Petviashvili (gKP) equation in (n + 1) dimensions. Based on the comprehensive three-wave methodology and the Hirota's bilinear technique, the gKP equation is meticulously examined. By means of symbolic computation, a number of three-wave solutions are derived. Applying the Lie symmetry approach to the governing equation enables the determination of symmetry reduction, which aids in the reduction of the dimensionality of the said equation. Using symmetry reduction, we obtain the second order differential equation. By means of applying symmetry reduction, the second order differential equation is derived. The second order differential equation undergoes Galilean transformation to obtain a system of first order differential equations. The present study presents an analysis of bifurcation and sensitivity for a given dynamical system. Additionally, when an external force impacts the underlying dynamic system, its behavior resembles quasi-periodic phenomena. The presence of quasi-periodic patterns are identified using chaos detecting tools. These findings represent a novel contribution to the studied equation and significantly advance our understanding of dynamics in nonlinear wave models.

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PubMed ID: 39190639

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ISSN: 1932-6203

Record 46 of 274

Title: An ADAR1 dsRBD3-PKR kinase domain interaction on dsRNA inhibits PKR activation

Author(s): Sinigaglia, K (Sinigaglia, Ketty); Cherian, A (Cherian, Anna); Du, QP (Du, Qiupei); Lacovich, V (Lacovich, Valentina); Vukic, D (Vukic, Dragana); Melicherová, J (Melicherova, Janka); Linhartova, P (Linhartova, Pavla); Zerad, L (Zerad, Lisa); Stejskal, S (Stejskal, Stanislav); Malik, R (Malik, Radek); Prochazka, J (Prochazka, Jan); Bondurand, N (Bondurand, Nadege); Sedlácek, R (Sedlacek, Radislav); O'Connell, MA (O'Connell, Mary A.); Keegan, LP (Keegan, Liam P.)

Source: CELL REPORTS **Volume:** 43 **Issue:** 8 **Article Number:** 114618 **DOI:** 10.1016/j.celrep.2024.114618 **Early Access Date:** AUG 2024 **Published Date:** 2024 AUG 27

Abstract: Adar null mutant mouse embryos die with aberrant double-stranded RNA (dsRNA)-driven interferon induction, and Adar Mavs double mutants, in which interferon induction is prevented, die soon after birth. Protein kinase R (Pkr) is aberrantly activated in Adar Mavs mouse pup intestines before death, intestinal crypt cells die, and intestinal villi are lost. Adar Mavs Eifak2 (Pkr) triple mutant mice rescue all defects and have longterm survival. Adenosine deaminase acting on RNA 1 (ADAR1) and PKR co-immunoprecipitate from cells, suggesting PKR inhibition by direct interaction. AlphaFold studies on an inhibitory PKR dsRNA binding domain (dsRBD)-kinase domain interaction before dsRNA binding and on an inhibitory ADAR1 dsRBD3PKR kinase domain interaction on dsRNA provide a testable model of the inhibition. Wild-type or editing- inactive human ADAR1 expressed in A549 cells inhibits activation of endogenous PKR. ADAR1 dsRNA binding is required for, but is not sufficient for, PKR inhibition. Mutating the ADAR1 dsRBD3-PKR contact prevents co-immunoprecipitation, ADAR1 inhibition of PKR activity, and co-localization of ADAR1 and PKR in cells.

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PubMed ID: 39146181

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Melicherova, Janka	GQQ-6545-2022	
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Linhartova (Musilova), Pavla	LTZ-4390-2024	0000-0002-8599-3413

ISSN: 2211-1247

Record 47 of 274

Title: Charge and Spin Transfer Dynamics in a Weakly Coupled Porphyrin Dimer

Author(s): Kopp, SM (Kopp, Sebastian M.); Redman, AJ (Redman, Ashley J.); Roncevic, I (Roncevic, Igor); Schröder, L (Schroder, Lisa); Bogani, L (Bogani, Lapo); Anderson, HL (Anderson, Harry L.); Timmel, CR (Timmel, Christiane R.)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 146 **Issue:** 31 **Pages:** 21476-21489 **DOI:** 10.1021/jacs.4c04186 **Early Access Date:** JUL 2024 **Published Date:** 2024 JUL 23

Abstract: The dynamics of electron and spin transfer in the radical cation and photogenerated triplet states of a tetramethylbiphenyl-linked zinc-porphyrin dimer were investigated, so as to test the relevant parameters for the design of a single-molecule spin valve and the creation of a novel platform for the photogeneration of high-multiplicity spin states. We used a combination of multiple techniques, including variable-temperature continuous wave EPR, pulsed proton electron-nuclear double resonance (ENDOR), transient EPR, and optical spectroscopy. The conclusions are further supported by density functional theory (DFT) calculations and comparison to reference compounds. The low-temperature cw-EPR and room-temperature near-IR spectra of the dimer monocation demonstrate that the radical cation is spatially localized on one side of the dimer at any point in time, not coherently delocalized over both porphyrin units. The EPR spectra at 298 K reveal rapid hopping of the radical spin density between both sites of the dimer via reversible intramolecular electron transfer. The hyperfine interactions are modulated by electron transfer and can be quantified using ENDOR spectroscopy. This allowed simulation of the variable-temperature cw-EPR spectra with a two-site exchange model and provided information on the temperature-dependence of the electron transfer rate. The electron transfer rates range from about 10.0 MHz at 200 K to about 53.9 MHz at 298 K. The activation enthalpies Delta double dagger H of the electron transfer were determined as Delta double dagger H = 9.55 kJ mol(-1) and Delta double dagger H = 5.67 kJ mol(-1) in a 1:1:1 solvent mixture of CD2Cl2/toluene-d(8)/THF-d(8) and in 2-methyltetrahydrofuran, respectively, consistent with a Robin-Day class II mixed valence compound. These results indicate that the interporphyrin electronic coupling in a tetramethylbiphenyl-linked porphyrin dimer is suitable for the backbone of a single-molecule spin valve. Investigation of the spin density distribution of the photogenerated triplet state of the Zn-porphyrin dimer reveals localization of the triplet spin density on a nanosecond time scale on one-half of the dimer at 20 K in 2-methyltetrahydrofuran and at 250 K in a polyvinylcarbazole film. This establishes the porphyrin dimer as a molecular platform for the formation of a localized, photogenerated triplet state on one porphyrin unit that is coupled to a second redox-active, ground-state porphyrin unit, which can be explored for the formation of high-multiplicity spin states.

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Record 48 of 274

Title: Tungsten wall cratering under high-velocity dust impacts: Influence of impact angle and temperature

Author(s): Dwivedi, P (Dwivedi, P.); Fraile, A (Fraile, A.); Polcar, T (Polcar, T.)

Source: JOURNAL OF NUCLEAR MATERIALS **Volume:** 600 **Article Number:** 155289 **DOI:** 10.1016/j.jnucmat.2024.155289 **Early Access Date:** JUL 2024 **Published Date:** 2024 NOV

Abstract: The integrity of plasma-facing components (PFCs) in fusion reactors is severely tested by high-velocity dust collisions, which occur during explosive events such as runaway electron terminations. These events can expel dust particles at velocities of 0.5 - 1 km/s in current fusion devices and potentially several km/s in advanced reactors like ITER and DEMO, leading to significant material erosion and damage. Given the limitations of existing models, which effectively address only low-velocity impacts, there is a critical need for improved modeling of high-velocity dust-wall interactions. This study utilizes molecular dynamics (MD) simulations to explore the effects of impact angle and target temperature on the interactions between tungsten (W) dust particles and W walls under extreme velocities ranging from 2.5 to 4.5 km/s. Our research focuses on analyzing the morphology of impact craters, and characteristics of ejecta across a range of impact angles (0 degrees degrees to 75 degrees) degrees) and with dislocation density for temperatures (300 to 3000 K). Our study reveals that the angle of impact and temperature almost exclusively determine the shape of the crater and the distribution of ejecta, highlighting the critical role of these factors in the dynamics of dust-wall interactions. Comparison with the experimental data obtained from Won-W impact tests shows a strong correlation with our theoretical predictions.

Accession Number: WOS:001274558600001

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ISSN: 0022-3115

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Record 49 of 274

Title: Similarities and Differences of Hydridic and Protonic Hydrogen Bonding

Author(s): Lamanec, M (Lamanec, Maximilian); Zienertova, J (Zienertova, Jitka); Spetko, M (Spetko, Matej); Nachtigallova, D (Nachtigallova, Dana); Hobza, P (Hobza, Pavel)

Source: CHEMPHYSCHEM **Volume:** 25 **Issue:** 17 **DOI:** 10.1002/cphc.202400403 **Early Access Date:** JUL 2024 **Published Date:** 2024 SEP 2

Abstract: Ab initio calculations were employed to investigate the interactions between selected electron-donating groups, characterized by M-H bonds (where M represents a transition metal and H denotes a hydridic hydrogen), and electron-accepting groups featuring both sigma- and pi-holes. The study utilized the omega B97X-D3BJ/def2-TZVPPD level of theory. Hydridic hydrogen complexes were found in all complexes with sigma- and pi-holes. A comparative analysis was conducted on the properties hydridic H-bond complexes, presented here and those studied previously, alongside an extended set of protonic H-bonds complexes. While the stabilization energies changes in M-H bond lengths, vibrational frequencies, intensities of the spectral bands, and charge transfer for these complexes are comparable, the nature of hydridic and protonic H-bonds fundamentally differ. In protonic H-bond complexes, the main stabilization forces arise from electrostatic contributions, while in hydridic H-bond complexes, dispersion energy, is the primary stabilization factor due to the excess of electrons and thus larger polarizability at hydridic H. The finding represents an important characteristic that distinguishes hydridic H-bonding from protonic H-bonds.
A standard hydrogen bond is formed between a protonic hydrogen possessing a partial positive charge and an electron donor. In contrast, a hydridic hydrogen bond is formed between a hydridic hydrogen bearing a partial negative charge and an electron acceptor. The characteristics of both types of hydrogen bonds, such as stabilization energy and red/blue shifts of the X-H stretching frequency, are very similar. image

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PubMed ID: 38771647

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Record 50 of 274

Title: Profiles of oxygen and titanium point defects in ferromagnetic TiO₂ films

Author(s): Nhu, TQ (Nhu, Tran Quynh); Friák, M (Friak, Martin); Miháliková, I (Mihalikova, Ivana); Kiaba, M (Kiaba, Michal); Hong, NH (Hong, Nguyen Hoa)

Source: JOURNAL OF PHYSICS D-APPLIED PHYSICS **Volume:** 57 **Issue:** 26 **Article Number:** 265302 **DOI:** 10.1088/1361-6463/ad3767 **Published Date:** 2024 JUL 5

Abstract: Experimentally it is shown that without any oxygen manipulation for TiO2, a strong room temperature ferromagnetism could be expected only in ultra-thin films, with the ideal thickness below 100 nm. Both bulks and nano-powders of TiO2 are diamagnetic, indicating that the surface and its nano-sublayers play very important roles in tailoring the magnetic properties in this type of compound. To shed a new light on the defect-related magnetism in the typical case of anatase TiO2 surfaces, we have performed a series of quantum-mechanical calculations for TiO2 slabs containing Ti or O vacancies in different distances from the (001) surface. The lowest formation energies were obtained for the Ti vacancies in the first sub-surface layer and the O vacancies within the surface. The computed magnetic states reflect complicated structural relaxations of atoms influenced by both the surface and vacant atomic positions. O atoms cannot contribute much to magnetic moment when Ti vacancies are isolated and far from the surface. Ti vacancies in TiO2 are only metastable. The formation energy of Ti interstitials is lower than for Ti vacancies since high-temperature annealing, especially with a lot of O-2 available that would fill up O-related defects, and as a result, eliminate most of Ti vacancies. Lower temperatures, less O-2, and shorter exposure times may enable not only partial elimination of Ti vacancies but also can facilitate their diffusion into different states of aggregations. In the ferromagnetic

films (i.e. thin films below 100 nm), it looks like that the O atoms are located closer to the Ti vacancies.

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Record 51 of 274

Title: Knot or not? Identifying unknotted proteins in knotted families with sequence-based Machine Learning model

Author(s): Sikora, M (Sikora, Maciej); Klimentova, E (Klimentova, Eva); Uchal, D (Uchal, Dawid); Sramkova, D (Sramkova, Denisa); Perlinska, AP (Perlinska, Agata P.); Nguyen, ML (Nguyen, Mai Lan); Korpacz, M (Korpacz, Marta); Malinowska, R (Malinowska, Roksana); Nowakowski, S (Nowakowski, Szymon); Rubach, P (Rubach, Pawel); Simecek, P (Simecek, Petr); Sulkowska, JI (Sulkowska, Joanna I.)

Source: PROTEIN SCIENCE **Volume:** 33 **Issue:** 7 **Article Number:** e4998 **DOI:** 10.1002/pro.4998 **Published Date:** 2024 JUL

Abstract: Knotted proteins, although scarce, are crucial structural components of certain protein families, and their roles continue to be a topic of intense research. Capitalizing on the vast collection of protein structure predictions offered by AlphaFold (AF), this study computationally examines the entire UniProt database to create a robust dataset of knotted and unknotted proteins. Utilizing this dataset, we develop a machine learning (ML) model capable of accurately predicting the presence of knots in protein structures solely from their amino acid sequences. We tested the model's capabilities on 100 proteins whose structures had not yet been predicted by AF and found agreement with our local prediction in 92% cases. From the point of view of structural biology, we found that all potentially knotted proteins predicted by AF can be classified only into 17 families. This allows us to discover the presence of unknotted proteins in families with a highly conserved knot. We found only three new protein families: UCH, DUF4253, and DUF2254, that contain both knotted and unknotted proteins, and demonstrate that deletions within the knot core could potentially account for the observed unknotted (trivial) topology. Finally, we have shown that in the majority of knotted families (11 out of 15), the knotted topology is strictly conserved in functional proteins with very low sequence similarity. We have conclusively demonstrated that proteins AF predicts as unknotted are structurally accurate in their unknotted configurations. However, these proteins often represent nonfunctional fragments, lacking significant portions of the knot core (amino acid sequence).

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PubMed ID: 38888487

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Record 52 of 274

Title: Strain-induced changes of electronic and optical properties of Zr-based MXenes

Author(s): Kalmár, J (Kalmar, Jiri); Karlick, F (Karlicky, Frantisek)

Source: JOURNAL OF APPLIED PHYSICS **Volume:** 135 **Issue:** 24 **Article Number:** 244302 **DOI:** 10.1063/5.0205991 **Published Date:** 2024 JUN 28

Abstract: Zr-based MXenes recently attracted attention because of its experimental preparation showing temperature stability, mechanical strength, and promising energy, sensoric, and electrochemistry applications. However, necessary theoretical predictions at a precise/predictive level are complicated due to essential excitonic features and strong electron correlation (i.e., a necessity to go beyond standard density functional theory, DFT). Contrary to the prevailing focus on oxygen-terminated MXenes and standard predictions of other Zr-based MXenes as conductors, based on the hybrid DFT and GW many-body perturbational theory, we were able to find seven different semiconductors (five of them for their equilibrium geometry and two others under slight tensile biaxial strain) in the case of two- and three-layered Zr2CT2 and Zr3C2T2 configurations with various terminations (T = O, F, S, Cl). We observed semiconductor-to-conductor transition induced by strain in the majority of such Zr-based MXenes at an experimentally achievable strain range. Furthermore, using the Bethe-Salpeter equation (BSE), we demonstrated that selected semiconducting Zr-based MXenes possess high optical absorption efficiency (20%-30%) in the visible light range, underscoring their potential in photonic applications. The high sensitivity of Zr-based MXenes to external conditions and functionalization combined with the thermal stability makes the materials promising for applications at operational temperatures in electronic and optical technologies.

Accession Number: WOS:001257947800009

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Record 53 of 274

Title: Chemical fixation of atmospheric CO₂ in tricopper(II)-carbonato complexes with tetradentate N-donor ligands: reactive intermediates, probable mechanisms, and catalytic and magneto-structural studies

Author(s): Jana, NC (Jana, Narayan Ch.); Sun, YC (Sun, Yu-Chen); Herchel, R (Herchel, Radovan); Nandy, R (Nandy, Rakhi); Brandao, P (Brandao, Paula); Bagh, B (Bagh, Bidraha); Wang, XY (Wang, Xin-Yi); Panja, A (Panja, Anangamohan)

Source: DALTON TRANSACTIONS **Volume:** 53 **Issue:** 27 **Pages:** 11514-11530 **DOI:** 10.1039/d4dt00503a **Early Access Date:** JUN 2024 **Published Date:** 2024 JUL 9

Abstract: In the present era, the fixation of atmospheric CO2 is of significant importance and plays a crucial role in maintaining the balance of carbon and energy flow within ecosystems. Generally, CO2 fixation is carried out by autotrophic organisms; however, the scientific community has paid substantial attention to execute this process in laboratory. In this report, we synthesized two carbonato-bridged trinuclear copper(ii) complexes, [Cu-3(L1)(3)(mu(3)-CO3)](ClO4)(3) (1) and [Cu-3(L2)(3)(mu(3)-CO3)](ClO4)(3) (2) via atmospheric fixation of CO2 starting with Cu(ClO4)(2)center dot 6H(2)O and easily accessible pyridine/pyrazine-based N-4 donor Schiff base ligands L1 and L2, respectively. Under

very similar reaction conditions, the ligand framework embedded with the phenolate moiety (HL3) fails to do so because of the reduction of the Lewis acidity of the metal center, inhibiting the formation of a reactive hydroxide bound copper(ii) species, which is required for the fixation of atmospheric CO2. X-ray crystal structures display that carbonate-oxygen atoms bridge three copper(ii) centers in mu(3)syn-anti disposition in 1 and 2, whereas [Cu(HL3)(ClO4)] (3) is a mononuclear complex. Interestingly, we also isolated an important intermediate of atmospheric CO2 fixation and structurally characterized it as an anti-anti mu(2) carbonato-bridged dinuclear copper(ii) complex, [Cu-2(L2)(2)(mu(2)-CO3)](ClO4)(2)center dot MeOH (2-I), providing an in-depth understanding of CO2 fixation in these systems. Variable temperature magnetic susceptibility measurement suggests ferromagnetic interactions between the metal centers in both 1 and 2, and the results have been further supported by DFT calculations. The catalytic efficiency of our synthesized complexes 1-3 was checked by means of catechol oxidase and phenoxazinone synthase-like activities. While complexes 1 and 2 showed oxidase-like activity for aerobic oxidation of o-aminophenol and 3,5-di-tert-butylcatechol, complex 3 was found to be feebly active. ESI mass spectrometry revealed that the oxidation reaction proceeds through the formation of complex-substrate intermediations and was further substantiated by DFT calculations. Moreover, active catalysts 1 and 2 were effectively utilized for the base-free oxidation of benzylic alcohols in the presence of air as a green and sustainable oxidant and catalytic amount of TEMPO in acetonitrile. Various substituted benzylic alcohols smoothly converted to their corresponding aldehydes under very mild conditions and ambient temperature. The present catalytic protocol showcases its environmental sustainability by producing minimal waste.

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ISSN: 1477-9226

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Record 54 of 274

Title: A Three-Grid High-Order Immersed Finite Element Method for the Analysis of CAD Models

Author(s): Febrianto, E (Febrianto, Eky); Sistek, J (Sistek, Jakub); Kus, P (Kus, Pavel); Kecman, M (Kecman, Matija); Cirak, F (Cirak, Fehmi)

Source: COMPUTER-AIDED DESIGN **Volume:** 173 **Article Number:** 103730 **DOI:** 10.1016/j.cad.2024.103730 **Early Access Date:** MAY 2024 **Published Date:** 2024 AUG

Abstract: The automated finite element analysis of complex CAD models using boundary -fitted meshes is rife with difficulties. Immersed finite element methods are intrinsically more robust but usually less accurate. In this work, we introduce an efficient, robust, high -order immersed finite element method for complex CAD models. Our approach relies on three adaptive structured grids: a geometry grid for representing the implicit geometry, a finite element grid for discretising physical fields and a quadrature grid for evaluating the finite element integrals. The geometry grid is a sparse VDB (Volumetric Dynamic B+ tree) grid that is highly refined close to physical domain boundaries. The finite element grid consists of a forest of octree grids distributed over several processors, and the quadrature grid in each finite element cell is an octree grid constructed in a bottom -up fashion. The resolution of the quadrature grid

ensures that finite element integrals are evaluated with sufficient accuracy and that any sub -grid geometric features, like small holes or corners, are resolved up to a desired resolution. The conceptual simplicity and modularity of our approach make it possible to reuse open -source libraries, i.e. openVDB and p4est for implementing the geometry and finite element grids, respectively, and BDDCML for iteratively solving the discrete systems of equations in parallel using domain decomposition. We demonstrate the efficiency and robustness of the proposed approach by solving the Poisson equation on domains described by complex CAD models and discretised with tens of millions of degrees of freedom. The solution field is discretised using linear and quadratic Lagrange basis functions.

Accession Number: WOS:001248243600002

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ISSN: 0010-4485

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Record 55 of 274

Title: AggreProt: a web server for predicting and engineering aggregation prone regions in proteins

Author(s): Planas-Iglesias, J (Planas-Iglesias, Joan); Borko, S (Borko, Simeon); Swiatkowski, J (Swiatkowski, Jan); Elias, M (Elias, Matej); Havlasek, M (Havlasek, Martin); Salamon, O (Salamon, Ondrej); Grakova, E (Grakova, Ekaterina); Kunka, A (Kunka, Antonin); Martinovic, T (Martinovic, Tomas); Damborsky, J (Damborsky, Jiri); Martinovic, J (Martinovic, Jan); Bednar, D (Bednar, David)

Source: NUCLEIC ACIDS RESEARCH **Volume:** 52 **Issue:** W1 **Pages:** W159-W169 **DOI:** 10.1093/nar/gkae420 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 27

Abstract: Recombinant proteins play pivotal roles in numerous applications including industrial biocatalysts or therapeutics. Despite the recent progress in computational protein structure prediction, protein solubility and reduced aggregation propensity remain challenging attributes to design. Identification of aggregation-prone regions is essential for understanding misfolding diseases or designing efficient protein-based technologies, and as such has a great socio-economic impact. Here, we introduce AggreProt, a user-friendly webserver that automatically exploits an ensemble of deep neural networks to predict aggregation-prone regions (APRs) in protein sequences. Trained on experimentally evaluated hexapeptides, AggreProt compares to or outperforms state-of-the-art algorithms on two independent benchmark datasets. The server provides per-residue aggregation profiles along with information on solvent accessibility and transmembrane propensity within an intuitive interface with interactive sequence and structure viewers for comprehensive analysis. We demonstrate AggreProt efficacy in predicting differential aggregation behaviours in proteins on several use cases, which emphasize its potential for guiding protein engineering strategies towards decreased aggregation propensity and improved solubility. The webserver is freely available and accessible at https://loschmidt.chemi.muni.cz/aggreprot/.
Graphical Abstract

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Record 56 of 274

Title: Nuclear patterns of phosphatidylinositol 4,5-and 3,4-bisphosphate revealed by super-resolution microscopy differ between the consecutive stages of RNA polymerase II transcription

Author(s): Hoboth, P (Hoboth, Peter); Sztacho, M (Sztacho, Martin); Hozák, P (Hozak, Pavel)

Source: FEBS JOURNAL **Volume:** 291 **Issue:** 19 **Pages:** 4240-4264 **DOI:** 10.1111/febs.17136 **Early Access Date:** MAY 2024 **Published Date:** 2024 OCT

Abstract: Phosphatidylinositol phosphates are powerful signaling molecules that orchestrate signaling and direct membrane trafficking in the cytosol. Interestingly, phosphatidylinositol phosphates also localize within the membrane-less compartments of the cell nucleus, where they participate in the regulation of gene expression. Nevertheless, current models of gene expression, which include condensates of proteins and nucleic acids, do not include nuclear phosphatidylinositol phosphates. This gap is partly a result of the missing detailed analysis of the subnuclear distribution of phosphatidylinositol phosphates and their relationships with gene expression. Here, we used quantitative dual-color direct stochastic optical reconstruction microscopy to analyze the nanoscale co-patterning between RNA polymerase II transcription initiation and elongation markers with respect to phosphatidylinositol 4,5- or 3,4-bisphosphate in the nucleoplasm and nuclear speckles and compared it with randomized data and cells with inhibited transcription. We found specific co-patterning of the transcription initiation marker P-S5 with phosphatidylinositol 4,5-bisphosphate in the nucleoplasm and with phosphatidylinositol 3,4-bisphosphate at the periphery of nuclear speckles. We showed the specific accumulation of the transcription elongation marker PS-2 and of nascent RNA in the proximity of phosphatidylinositol 3,4-bisphosphate associated with nuclear speckles. Taken together, this shows that the distinct spatial associations between the consecutive stages of RNA polymerase II transcription and nuclear phosphatidylinositol phosphates exhibit specificity within the gene expression compartments. Thus, in analogy to the cellular membranes, where phospholipid composition orchestrates signaling pathways and directs membrane trafficking, we propose a model in which the phospholipid identity of gene expression compartments orchestrates RNA polymerase II transcription.

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PubMed ID: 38734927

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Record 57 of 274

Title: Resonant Tip-Enhanced Raman Spectroscopy of a Single-Molecule Kondo System

Author(s): Ferreira, RCD (Ferreira, Rodrigo Cezar de Campos); Sagwal, A (Sagwal, Amandeep); Dolezal, J (Dolezal, Jiri); Canola, S (Canola, Sofia); Merino, P (Merino, Pablo); Neuman, T (Neuman, Tomas); Svec, M (Svec, Martin)

Source: ACS NANO **Volume:** 18 **Issue:** 20 **Pages:** 13164-13170 **DOI:** 10.1021/acsnano.4c02105 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 7

Abstract: Tip-enhanced Raman spectroscopy (TERS) under ultrahigh vacuum and cryogenic conditions enables exploration of the relations between the adsorption geometry, electronic state, and vibrational fingerprints of individual molecules. TERS capability of reflecting spin states in open-shell molecular configurations is yet unexplored. Here, we use the tip of a scanning probe microscope to lift a perylene-3,4,9,10-tetracarboxylic dianhydride (PTCDA) molecule from a metal surface to bring it into an open-shell spin one-half anionic state. We reveal a correlation between the appearance of a Kondo resonance in differential conductance spectroscopy and concurrent characteristic changes captured by the TERS measurements. Through a detailed investigation of various adsorbed and tip-contacted PTCDA scenarios, we infer that the Raman scattering on suspended PTCDA is resonant with a higher excited state. Theoretical simulation of the vibrational spectra enables a precise assignment of the individual TERS peaks to high-symmetry Ag modes, including the fingerprints of the observed spin state. These findings highlight the potential of TERS in capturing complex interactions between charge, spin, and photophysical properties in nanoscale molecular systems and suggest a pathway for designing single-molecule spin-optical devices.

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PubMed ID: 38711331

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Record 58 of 274

Title: Intergeneric hybrid origin of the invasive tetraploid Cirsium vulgare

Author(s): Bures, P (Bures, P.); Del Guacchio, E (Del Guacchio, E.); Smerda, J (Smerda, J.); Özcan, M (Ozcan, M.); Bliznaková, P (Bliznakova, P.); Vavrinec, M (Vavrinec, M.); Michálková, E (Michalkova, E.); Vesely, P (Vesely, P.); Veselá, K (Vesela, K.); Zedek, F (Zedek, F.)

Source: PLANT BIOLOGY **Volume:** 26 **Issue:** 5 **Pages:** 749-763 **DOI:** 10.1111/plb.13653 **Early Access Date:** MAY 2024 **Published Date:** 2024 AUG

Abstract: center dot The invasive tetraploid Cirsium vulgare hybridizes with both Cirsium and Lophiolepis. Its conflicted position in molecular phylogenies, and its peculiar combination of morphological, anatomical, and genomic features that are alternatively shared with representatives of Cirsium or Lophiolepis, strongly suggest its intergeneric hybrid origin. center dot Genetic relationships of C. vulgare (8 samples) with genus Lophiolepis (11 species) and other representatives of genus Cirsium (12 species) were evaluated using restriction site-associated DNA sequencing (RADseq) and examined

using analytical and imaging approaches, such as NeighborNet, Heatmap, and STRUCTURE, to identify nuclear genomes admixture. Estimation of the intensity of spontaneous hybridization within and between Cirsium and Lophiolepis was based on herbarium revisions and published data for all reported hybrids pertinent to taxa currently included in Cirsium or Lophiolepis. center dot The genome of any examined Cirsium species is more similar to C. vulgare than to any Lophiolepis species, and vice versa. The nuclear genome of the tetraploid C. vulgare is composed of two equivalent parts, each attributable either to Lophiolepis or to Cirsium; the organellar RADseq data clustered C. vulgare with the genus Cirsium. Spontaneous hybridization between Cirsium and Lophiolepis is significantly less intensive than within these genera. center dot Our analyses provide compelling evidence that the invasive species C. vulgare has an allotetraploid intergeneric origin, with the maternal parent from Cirsium and the paternal from Lophiolepis. For the purpose of delimiting monophyletic genera, we propose keeping Lophiolepis separate from Cirsium and segregating C. vulgare into the hybridogenous genus Ascalea.

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PubMed ID: 38704835

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ISSN: 1435-8603

eISSN: 1438-8677

Record 59 of 274

Title: Nanoparticle induced fusion of lipid membranes

Author(s): Blasco, S (Blasco, Sofia); Sukeník, L (Sukenik, Lukas); Vácha, R (Vacha, Robert)

Source: NANOSCALE **Volume:** 16 **Issue:** 21 **DOI:** 10.1039/d4nr00591k **Early Access Date:** APR 2024 **Published Date:** 2024 MAY 30

Abstract: Membrane fusion is crucial for infection of enveloped viruses, cellular transport, and drug delivery via liposomes. Nanoparticles can serve as fusogenic agents facilitating such membrane fusion for direct transmembrane transport. However, the underlying mechanisms of nanoparticle-induced fusion and the ideal properties of such nanoparticles remain largely unknown. Here, we used molecular dynamics simulations to investigate the efficacy of spheroidal nanoparticles with different size, prolateness, and ligand interaction strengths to enhance fusion between vesicles. By systematically varying nanoparticle properties, we identified how each parameter affects the fusion process and determined the optimal parameter range that promotes fusion. These findings provide valuable insights for the design and optimization of fusogenic nanoparticles with potential biotechnological and biomedical applications.
We found that the optimal fusogenic nanoparticle is able to form a stalk but does not overstabilize it, facilitating the opening of a fusion pore.

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PubMed ID: 38679949

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Record 60 of 274

Title: Characterization of Mycoviruses in Armillaria ostoyae and A. cepistipes in the Czech Republic

Author(s): Walterová, L (Walterova, Lucie); Botella, L (Botella, Leticia); Hejna, O (Hejna, Ondrej); de la Peña, M (de la Pena, Marcos); Tonka, T (Tonka, Tomas); Curn, V (Curn, Vladislav)

Source: VIRUSES-BASEL **Volume:** 16 **Issue:** 4 **Article Number:** 610 **DOI:** 10.3390/v16040610 **Published Date:** 2024 APR

Abstract: Members of the genus Armillaria are widespread forest pathogens against which effective protection has not yet been developed. Due to their longevity and the creation of large-scale cloning of Armillaria individuals, the use of mycoviruses as biocontrol agents (BCAs) against these pathogens could be an effective alternative. This work describes the detection and characterization of viruses in Armillaria spp. collected in the Czech Republic through the application of stranded total RNA sequencing. A total of five single-stranded RNA viruses were detected in Armillaria ostoyae and A. cepistipes, including viruses of the family Tymoviridae and four viruses belonging to the recently described "ambivirus" group with a circular ambisense genome arrangement. Both hammerhead (HHRz) and hairpin (HpRz) ribozymes were detected in all the ambiviricot sequences. Armillaria viruses were compared through phylogenetic analysis and confirmed their specific host by direct RT-PCR. One virus appears to infect both Armillaria species, suggesting the occurrence of interspecies transmission in nature.

Accession Number: WOS:001211450300001

PubMed ID: 38675951

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eISSN: 1999-4915

Record 61 of 274

Title: High-velocity dust impacts in plasma facing materials: Insights from molecular dynamics simulations

Author(s): Dwivedi, P (Dwivedi, Prashant); Fraile, A (Fraile, Alberto); Polcar, T (Polcar, Tomas)

Source: JOURNAL OF NUCLEAR MATERIALS **Volume:** 594 **Article Number:** 155042 **DOI:** 10.1016/j.jnucmat.2024.155042 **Early Access Date:** MAR 2024 **Published Date:** 2024 JUN

Abstract: This research investigates the interaction between high-speed tungsten (W) dust and plasma - facing components (PFCs) in fusion reactors, particularly focusing on W walls. Through molecular dynamics (MD) simulations, the study covers a broad spectrum of W dust velocities to evaluate their effect on wall materials with various crystal orientations. We found that high-speed impacts cause considerable damage, including sputtering, degradation, and deformation. The study introduces a damage model derived from experimental and simulation data that reveals the patterns and mechanisms of damage caused by dust impacts. The proposed model significantly improves our understanding of dust - wall interactions and underscores the importance of MD simulations as a reliable technique for exploring such phenomena in the challenging conditions of fusion devices. These insights are crucial to predict and mitigate damage to PFCs, helping to develop more resilient and efficient components. Overall, the

research offers valuable knowledge on the atomic -level dynamics of dust impacts and represents a notable advancement in the durability and efficiency of materials used in fusion energy technologies.

Accession Number: WOS:001221201200001

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ISSN: 0022-3115

eISSN: 1873-4820

Record 62 of 274

Title: ViCTORIA project: The LOFAR view of environmental effects in Virgo cluster star-forming galaxies

Author(s): Edler, HW (Edler, H. W.); Roberts, ID (Roberts, I. D.); Boselli, A (Boselli, A.); de Gasperin, F (de Gasperin, F.); Heesen, V (Heesen, V.); Brüggen, M (Brueggen, M.); Ignesti, A (Ignesti, A.); Gajovic, L (Gajovic, L.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 683 **Article Number:** A149 **DOI:** 10.1051/0004-6361/202348301 **Published Date:** 2024 MAR 18

Abstract: Context. Environmental effects such as ram pressure stripping (RPS) shape the evolution of galaxies in dense regions. Aims. We used the nearby Virgo cluster as a laboratory to study the environmental effects on the nonthermal components of star-forming galaxies. Methods. We constructed a sample of 17 RPS galaxies in the Virgo cluster and a statistical control sample of 119 nearby galaxies from the Herschel Reference Survey. All objects in these samples were detected in LOFAR 144 MHz observations and come with H alpha and/or far-UV star formation rate (SFR) estimates. Results. We derived the radio-SFR relations, confirming a clearly super-linear slope of approximate to 1.4. We found that Virgo cluster RPS galaxies have radio luminosities that are a factor of 2-3 larger than galaxies in our control sample. We also investigated the total mass-spectral index relation, where we found a relation for the Virgo cluster RPS galaxies that is shifted to steeper spectral index values by 0.17 +/- 0.06. Analyzing the spatially resolved ratio between the observed and the expected radio emission based on the hybrid near-UV + 100 mu m SFR surface density, we generally observed excess radio emission all across the disk with the exception of a few leading-edge radio-deficient regions. Conclusions. The radio excess and the spectral steepening for the RPS sample could be explained by an increased magnetic field strength if the disk-wide radio enhancement is due to projection effects. For the galaxies that show the strongest radio excesses (NGC 4330, NGC 4396 and NGC 4522), a rapid decline in the SFR (t(quench) <= 100 Myr) could be an alternative explanation. We disfavor shock acceleration of electrons as a cause for the radio excess since it cannot easily explain the spectral steepening and radio morphology.

Accession Number: WOS:001186725700012

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Record 63 of 274

Title: Charge Regulation Triggers Condensation of Short Oligopeptides to Polyelectrolytes

Author(s): Pineda, SP (Pineda, Sebastian P.); Stano, R (Stano, Roman); Murmiliuk, A (Murmiliuk, Anastasiia); Blanco, PM (Blanco, Pablo M.); Montes, P (Montes, Patricia); Tosner, Z (Tosner, Zdenek); Groborz, O (Groborz, Ondrej); Pánek, J (Panek, Jiri); Hruby, M (Hruby, Martin); Stepánek, M (Stepanek, Miroslav); Kosovan, P (Kosovan, Peter)

Source: JACS AU **Volume:** 4 **Issue:** 5 **Pages:** 1775-1785 **DOI:** 10.1021/jacsau.3c00668 **Early Access Date:** MAR 2024 **Published Date:** 2024 MAR 13

Abstract: Electrostatic interactions between charged macromolecules are ubiquitous in biological systems, and they are important also in materials design. Attraction between oppositely charged molecules is often interpreted as if the molecules had a fixed charge, which is not affected by their interaction. Less commonly, charge regulation is invoked to interpret such interactions, i.e., a change of the charge state in response to a change of the local environment. Although some theoretical and simulation studies suggest that charge regulation plays an important role in intermolecular interactions, experimental evidence supporting such a view is very scarce. In the current study, we used a model system, composed of a long polyanion interacting with cationic oligolysines, containing up to 8 lysine residues. We showed using both simulations and experiments that while these lysines are only weakly charged in the absence of the polyanion, they charge up and condense on the polycations if the pH is close to the pK a of the lysine side chains. We show that the lysines coexist in two distinct populations within the same solution: (1) practically nonionized and free in solution; (2) highly ionized and condensed on the polyanion. Using this model system, we demonstrate under what conditions charge regulation plays a significant role in the interactions of oppositely charged macromolecules and generalize our findings beyond the specific system used here.

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PubMed ID: 38818083

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eISSN: 2691-3704

Record 64 of 274

Title: Heteromorphic ZZ/ZW sex chromosomes sharing gene content with mammalian XX/XY are conserved in Madagascan chameleons of the genus Furcifer

Author(s): Rovatsos, M (Rovatsos, Michail); Mazzoleni, S (Mazzoleni, Sofia); Augstenová, B (Augstenova, Barbora); Altmanová, M (Altmanova, Marie); Velensky, P (Velensky, Petr); Glaw, F (Glaw, Frank); Sanchez, A (Sanchez, Antonio); Kratochvíl, L (Kratochvil, Lukas)

Source: SCIENTIFIC REPORTS **Volume:** 14 **Issue:** 1 **Article Number:** 4898 **DOI:** 10.1038/s41598-024-55431-9 **Published Date:** 2024 FEB 28

Abstract: Chameleons are well-known lizards with unique morphology and physiology, but their sex determination has remained poorly studied. Madagascan chameleons of the genus Furcifer have cytogenetically distinct Z and W sex chromosomes and occasionally Z(1)Z(1)Z(2)Z(2)/Z(1)Z(2)W multiple neo-sex chromosomes. To identify the gene content of their sex chromosomes, we microdissected and sequenced the sex chromosomes of F. oustaleti (ZZ/ZW) and F. pardalis (Z(1)Z(1)Z(2)Z(2)/Z(1)Z(2)W). In addition, we sequenced the genomes of a male and a female of F. lateralis (ZZ/ZW) and F. pardalis and performed a comparative coverage analysis between the sexes. Despite the notable heteromorphy and distinctiveness in heterochromatin content, the Z and W sex chromosomes share approximately 90% of their gene content. This finding demonstrates poor correlation of the degree of differentiation of sex chromosomes at the cytogenetic and gene level. The test of homology based on the comparison of gene copy number variation revealed that female heterogamety with differentiated sex chromosomes remained stable in the genus Furcifer for at least 20 million years. These chameleons co-opted for the role of sex chromosomes the same genomic region as viviparous mammals, lacertids and geckos of the genus Paroedura, which makes these groups excellent model for studies of convergent and divergent evolution of sex chromosomes.

Accession Number: WOS:001178172300011

PubMed ID: 38418601

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ISSN: 2045-2322

Record 65 of 274

Title: Anisotropy Parameters for Two-Color Photoionization Phases in Randomly Oriented Molecules: Theory and Experiment in Methane and Deuteromethane

Author(s): Ertel, D (Ertel, Dominik); Busto, D (Busto, David); Makos, I (Makos, Ioannis); Schmoll, M (Schmoll, Marvin); Benda, J (Benda, Jakub); Bragheri, F (Bragheri, Francesca); Osellame, R (Osellame, Roberto); Lindroth, E (Lindroth, Eva); Patchkovskii, S (Patchkovskii, Serguei); Masín, Z (Masin, Zdenek); Sansone, G (Sansone, Giuseppe)

Source: JOURNAL OF PHYSICAL CHEMISTRY A **Volume:** 128 **Issue:** 9 **Pages:** 1685-1697 **DOI:** 10.1021/acs.jpca.3c06759 **Early Access Date:** FEB 2024 **Published Date:** 2024 FEB 23

Abstract: We present combined theoretical and experimental work investigating the angle-resolved phases of the photoionization process driven by a two-color field consisting of an attosecond pulse train and an infrared pulse in an ensemble of randomly oriented molecules. We derive a general form for the two-color photoelectron (and time-delay) angular distribution valid also in the case of chiral molecules and when relative polarizations of the photons contributing to the attosecond photoelectron interferometer differ. We show a comparison between the experimental data and theoretical predictions in an ensemble of methane and deuteromethane molecules, discussing the effect of nuclear dynamics on the

photoionization phases. Finally, we demonstrate that the oscillating component and the phase of the two-color signal can be fitted by using complex asymmetry parameters, in perfect analogy to the atomic case.

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PubMed ID: 38394372

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ISSN: 1089-5639

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Record 66 of 274

Title: A chromosome arm from Thinopyrum intermedium x Thinopyrum ponticum hybrid confers increased tillering and yield potential in wheat

Author(s): Türkösi, E (Turkosi, Edina); Szakács, É (Szakacs, Eva); Ivanizs, L (Ivanizs, Laszlo); Farkas, A (Farkas, Andras); Gaál, E (Gaal, Eszter); Said, M (Said, Mahmoud); Darkó, É (Darko, Eva); Cséplo, M (Cseplo, Monika); Mikó, P (Miko, Peter); Dolezel, J (Dolezel, Jaroslav); Molnár-Láng, M (Molnar-Lang, Marta); Molnár, I (Molnar, Istvan); Kruppa, K (Kruppa, Klaudia)

Source: MOLECULAR BREEDING **Volume:** 44 **Issue:** 2 **Article Number:** 7 **DOI:** 10.1007/s11032-024-01439-y **Published Date:** 2024 FEB

Abstract: Tiller number is a key component of wheat plant architecture having a direct impact on grain yield. Because of their viability, biotic resistance, and abiotic stress tolerance, wild relative species are a valuable gene source for increasing wheat genetic diversity, including yield potential. Agropyron glael, a perennial hybrid of Thinopyrum intermedium and Th. ponticum, was created in the 1930s. Recent genome analyses identified five evolutionarily distinct subgenomes (J, J(st), J(vs), J (R), and St), making A. glael an important gene source for transferring useful agronomical traits into wheat. During a bread wheat x A. glael crossing program, a genetically stable translocation line, WT153397, was developed. Sequential in situ hybridizations (McGISH) with J-, St-, and D-genomic DNA probes and pSc119.2, Afa family, pTa71, and (GAA)(7) DNA repeats, as well as molecular markers specific for the wheat 6D chromosome, revealed the presence of a 6DS.6J(vs) Robertsonian translocation in the genetic line. Field trials in low-input and high-input breeding nurseries over four growing seasons demonstrated the Agropyron chromosome arm's high compensating ability for the missing 6DL, as spike morphology and fertility of WT153397 did not differ significantly from those of wheat parents, Mv9kr1 and 'Mv Karizma.' Moreover, the introgressed 6J(vs) chromosome arm significantly increased the number of productive tillers, resulting in a significantly higher grain yield potential compared to the parental wheat cultivars. The translocated chromosome could be highly purified by flow cytometric sorting due to the intense fluorescent labeling of (GAA)(7) clusters on the Thinopyrum chromosome arm, providing an opportunity to use chromosome genomics to identify Agropyron gene variant(s) responsible for the tillering capacity. The translocation line WT153397 is an important genetic stock for functional genetic studies of tiller formation and useful breeding material for increasing wheat yield potential. The study also discusses the use of the translocation line in wheat breeding.

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PubMed ID: 38263978

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Record 67 of 274

Title: Lewis Acidic Aluminosilicates: Synthesis, ²⁷Al MQ/MAS NMR, and DFT-Calculated ²⁷Al NMR Parameters

Author(s): Kejik, M (Kejik, Martin); Brus, J (Brus, Jiri); Jeremias, L (Jeremias, Lukas); Simonikova, L (Simonikova, Lucie); Moravec, Z (Moravec, Zdenek); Kobera, L (Kobera, Libor); Styskalik, A (Styskalik, Ales); Barnes, CE (Barnes, Craig E.); Pinkas, J (Pinkas, Jiri)

Source: INORGANIC CHEMISTRY **Volume:** 63 **Issue:** 5 **Pages:** 2679-2694 **DOI:** 10.1021/acs.inorgchem.3c04035 **Published Date:** 2024 JAN 25

Abstract: Porous aluminosilicates are functional materials of paramount importance as Lewis acid catalysts in the synthetic industry, yet the participating aluminum species remain poorly studied. Herein, a series of model aluminosilicate networks containing [L-AlO3] (L = THF, Et3N, pyridine, triethylphosphine oxide (TEPO)) and [AlO4]- centers were prepared through nonhydrolytic sol-gel condensation reactions of the spherosilicate building block (Me3Sn)(8)Si8O20 with L-AlX3 (X = Cl, Me, Et) and [Me4N] [AlCl4] compounds in THF or toluene. The substoichiometric dosage of the Al precursors ensured complete condensation and uniform incorporation, with the bulky spherosilicate forcing a separation between neighboring aluminum centers. The materials were characterized by H-1, C-13, Al-27, Si-29, and P-31 MAS NMR and FTIR spectroscopies, ICP-OES, gravimetry, and N2 adsorption porosimetry. The resulting aluminum centers were resolved by Al-27 TQ/MAS NMR techniques and assigned based on their spectroscopic parameters obtained by peak fitting (delta(iso), C Q, eta) and their correspondence to the values calculated on model structures by DFT methods. A clear correlation between the decrease in the symmetry of the Al centers and the increase of the observed C Q was established with values spanning from 4.4 MHz for distorted [AlO4](-) to 15.1 MHz for [THF-AlO3]. Products containing exclusively [TEPO-AlO3] or [AlO4](-) centers could be obtained (single-site materials). For L = THF, Et3N, and pyridine, the [AlO4](-) centers were formed together with the expected [L-AlO3] species, and a viable mechanism for the unexpected emergence of [AlO4]- was proposed.

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PubMed ID: 38271593

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ISSN: 0020-1669

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Record 68 of 274

Title: The ghost of past climate acting on present-day plant diversity: Lessons from a climate-based delimitation of the tropical alpine ecosystem

Author(s): Kandziora, M (Kandziora, Martha); Gorospe, JM (Gorospe, Juan M.); Salomon, L (Salomon, Luciana); Vasquez, DLA (Vasquez, Diana L. A.); Vargas, MP (Vargas, Maria Pinilla); Kolar, F (Kolar, Filip); Sklenar, P (Sklenar, Petr); Schmickl, R (Schmickl, Roswitha)

Source: JOURNAL OF SYSTEMATICS AND EVOLUTION **Volume:** 62 **Issue:** 2 **Special Issue:** SI **Pages:** 275-290 **DOI:** 10.1111/jse.13048 **Early Access Date:** JAN 2024 **Published Date:** 2024 MAR

Abstract: Habitat stability is important for maintaining biodiversity by preventing species extinction, but this stability is being challenged by climate change. The tropical alpine ecosystem is currently one of the ecosystems most threatened by global warming, and the flora close to the permanent snow line is at high risk of extinction. The tropical alpine ecosystem, found in South and Central America, Malesia and Papuasia, Africa, and Hawaii, is of relatively young evolutionary age, and it has been exposed to changing climates since its origin, particularly during the Pleistocene. Estimating habitat loss and gain between the Last Glacial Maximum (LGM) and the present allows us to relate current biodiversity to past changes in climate and habitat stability. In order to do so, (i) we developed a unifying climate-based delimitation of tropical alpine regions across continents, and (ii) we used this delimitation to assess the degree of habitat stability, that is, the overlap of suitable areas between the LGM and the present, in different tropical alpine regions. Finally, we discuss the link between habitat stability and tropical alpine plant diversity. Our climate-based delimitation approach can be easily applied to other ecosystems using our developed code, facilitating macro-comparative studies of habitat dynamics through time.
Using a climate-based delimitation to compare the extent of tropical alpine areas between the present and during the last glacial maximum permits us to estimate the degree of habitat stability. This new approach facilitates macro-comparative studies of habitat dynamics through time.image

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Record 69 of 274

Title: Interplay of EXO70 and MLO proteins modulates trichome cell wall composition and susceptibility to powdery mildew

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Source: PLANT CELL **DOI:** 10.1093/plcell/koad319 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN 22

Abstract: Exocyst component of 70-kDa (EXO70) proteins are constituents of the exocyst complex implicated in vesicle tethering during exocytosis. MILDEW RESISTANCE LOCUS O (MLO) proteins are plant-specific calcium channels and some MLO isoforms enable fungal powdery mildew pathogenesis. We here detected an unexpected phenotypic overlap of Arabidopsis thaliana exo70H4 and mlo2 mlo6 mlo12 triple mutant plants regarding the biogenesis of leaf trichome secondary cell walls. Biochemical and Fourier transform infrared spectroscopic analyses corroborated deficiencies in the composition of trichome cell walls in these mutants. Transgenic lines expressing fluorophore-tagged EXO70H4 and MLO exhibited extensive colocalization of these proteins. Furthermore, mCherry-EXO70H4 mislocalized in trichomes of the mlo triple mutant and, vice versa, MLO6-GFP mislocalized in trichomes of the exo70H4 mutant. Expression of GFP-marked PMR4 callose synthase, a known cargo of EXO70H4-dependent exocytosis, revealed reduced cell wall delivery of GFP-PMR4 in trichomes of mlo triple mutant plants. In vivo protein-protein interaction assays in plant and yeast cells uncovered isoform-preferential interactions between EXO70.2 subfamily members and MLO proteins. Finally, exo70H4 and mlo6 mutants, when combined, showed synergistically enhanced resistance to powdery mildew attack. Taken together, our data point to an isoform-specific interplay of EXO70 and MLO proteins in the modulation of trichome cell wall biogenesis and powdery mildew susceptibility. Shared trichome- and defense-related mutant phenotypes, subcellular colocalization, and isoform-preferential protein-protein interaction indicate interplay of EXO70 and MLO proteins in focal secretion.

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PubMed ID: 38124479

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ISSN: 1040-4651

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Record 70 of 274

Title: Nearly (?) sterile avian egg in a passerine bird

Author(s): Tesicky, M (Tesicky, Martin); Schmiedová, L (Schmiedova, Lucie); Krajzingrová, T (Krajzingrova, Tereza); Samblas, MG (Samblas, Mercedes Gomez); Bauerová, P (Bauerova, Petra); Kreisinger, J (Kreisinger, Jakub); Vinkler, M (Vinkler, Michal)

Source: FEMS MICROBIOLOGY ECOLOGY **Volume:** 100 **Issue:** 1 **Article Number:** fiad164 **DOI:** 10.1093/femsec/fiad164 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN 16

Abstract: During early ontogeny, microbiome affects development of the gastrointestinal tract, immunity, and survival in vertebrates. Bird eggs are thought to be (1) initially sterile (sterile egg hypothesis) and (2) colonized after oviposition through horizontal trans-shell migration, or (3) initially seeded with bacteria by vertical transfer from mother oviduct. To date, however, little empirical data illuminate the contribution of these mechanisms to gut microbiota formation in avian embryos. We investigated microbiome of the egg content (day 0; E0-egg), embryonic gut at day 13 (E13) and female faeces in a free-living passerine, the great tit (Parus major), using a methodologically advanced procedure combining 16S rRNA gene sequencing and microbe-specific qPCR assays. Our metabarcoding revealed that the avian egg is (nearly) sterile, but acquires a slightly richer microbiome during the embryonic development. Of the three potentially pathogenic bacteria targeted by qPCR, only Dietzia was found in E0-egg (yet also in negative controls), E13 gut and female samples, which might indicate possible vertical transfer. Unlike in poultry, we have shown that major bacterial colonization of the gut in passerines does not occur before hatching. We emphasize that protocols that carefully check for environmental contamination are critical in studies with low-bacterial biomass samples.
The eggs of great tits are nearly sterile when they are laid and are first colonised during embryonic development. Our results indicate that diversified microbial communities form in passerine birds after hatching.

Accession Number: WOS:001146416500002

PubMed ID: 38115624

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Record 71 of 274

Title: Diethyl ether anaesthesia inhibits de-etiolation of barley seedlings by locking them in intermediate skoto-photomorphogenetic state

Author(s): Pavlovic, A (Pavlovic, Andrej); Kopecna, M (Kopecna, Martina); Hlouskova, L (Hlouskova, Lucie); Koller, J (Koller, Jana); Hrivnacky, M (Hrivnacky, Martin); Ilik, P (Ilik, Petr); Bartos, J (Bartos, Jan)

Source: PHYSIOLOGIA PLANTARUM **Volume:** 176 **Issue:** 1 **Article Number:** e14144 **DOI:** 10.1111/ppl.14144 **Published Date:** 2024 JAN

Abstract: Light is an essential environmental signal for plant development called photomorphogenesis. Here, we show that diethyl ether anaesthesia inhibits the de-etiolation process in barley (Hordeum vulgare) seedlings. Illuminated seedlings exposed to diethyl ether accumulated significantly less chlorophylls and chlorophyll-binding proteins, and exhibited reduced maximum quantum yield of photosystem II photochemistry (Fv/Fm). Although the direct effect of light necessary for the greening process, i.e. for the photoreduction of protochlorophyllide (Pchlide) to chlorophyllide (Chlide) catalysed by light-dependent protochlorophyllide oxidoreductase A (PORA), was not inhibited, the RNA-seq and qPCR analyses showed that light-induced expression of photosynthesis-associated nuclear genes (PhANGs) and genes encoding enzymes for chlorophyll biosynthesis were attenuated. On the other hand, transcription of chloroplast-encoded genes was not negatively affected by diethyl ether treatment during greening. Among the genes negatively regulated by light, PORA and PHYA were only slightly affected by diethyl ether. The effect of diethyl ether was fully reversible and, after its removal, the greening process was fully restored. Our data indicate that diethyl ether had two effects on greening: i) it inhibited the expression of PhANGs and chlorophyll biosynthesis-related genes irrespective of light conditions, ii) it blocked the light-induced expression of these genes and greening process of etiolated seedlings. Our study indicates that diethyl ether affects plastid biogenesis, which alters the orchestration of negative and positive regulators affecting phytochrome and/or retrograde signalling and does not allow expression of PhANGs. Thus, the plants are locked in an intermediate skoto-photomorphogenetic state in the light.

Accession Number: WOS:001142148500001

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ISSN: 0031-9317

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Record 72 of 274

Title: A phylogenomic monograph of West-Palearctic Nomada (Hymenoptera: Apidae)

Author(s): Straka, J (Straka, Jakub); Benda, D (Benda, Daniel); Policarová, J (Policarova, Jana); Astapenková, A (Astapenkova, Alena); Wood, TJ (Wood, Thomas J.); Bossert, S (Bossert, Silas)

Source: INSECT SYSTEMATICS AND DIVERSITY **Volume:** 8 **Issue:** 1 **Article Number:** 1 **DOI:** 10.1093/isd/ixad024 **Published Date:** 2024 JAN 1

Abstract: We reconstruct the phylogeny of the most speciose genus of cuckoo bees, genus Nomada Scopoli, 1770, using 221 species from throughout its distribution, yet with a strong emphasis on the West Palearctic. For phylogenetic reconstruction, we sequenced ultraconserved elements, allowing robust phylogenetic estimates with both concatenation and coalescent-based methods. By integrating extensive information on Nomada host records, we study macroevolutionary patterns of host associations, transitions, and phylogenetic conservatism. Using Bayesian divergence time estimates, we assess the historical biogeography of the genus, focusing on the West Palearctic. Our results show that Nomada likely originated in the Eastern Mediterranean and Near Eastern region, and likely expanded its range to a near-global distribution from there. We recovered long-standing phylogenetic conservatism in the host usage of Nomada and provided strong statistical evidence for an ancestral host association with Andrena and its most recent common ancestor. However, host transitions occurred multiple times independently in the natural history of Nomada, and species of the genus are brood parasites in at least 5 genera and 4 different families of bees in the Old World. At last, we systematically revise the taxonomy of the Old

World Nomada by integrating morphological study with our well-supported phylogenetic estimates. We re-establish the genus Acanthonomada Schwarz, 1966, stat. res., as a distinct, second genus in the tribe Nomadini. We recognize 13 subgenera for Nomada, 9 of which are described as new: Afronomada Straka and Bossert, subgen. nov., Colliculla Straka, subgen. nov., Gestamen Straka, subgen. nov., Hungias Straka, subgen. nov., Mininomada Straka, subgen. nov., Nomacolla Straka, subgen. nov., Nomonosa Straka, subgen. nov., Plumada Straka, subgen. nov., and Profuga Straka, subgen. nov. Aside from the subgenus Nomada s.s., we reinstitute 3 previously synonymized subgenera: Heminomada Cockerell, 1902, stat. res., Holonomada Robertson, 1903, stat. res., and Hypochrotaenia Holmberg, 1886 stat. res. A total of 15 subgeneric names are formally synonymized with the newly established subgeneric concepts. Graphical Abstract

Accession Number: WOS:001137016000001

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Straka, Jakub	A-7215-2012	0000-0002-8987-1245

eISSN: 2399-3421

Record 73 of 274

Title: LOFAR high-band antenna observations of the Perseus cluster The discovery of a giant radio halo

Author(s): van Weeren, RJ (van Weeren, R. J.); Timmerman, R (Timmerman, R.); Vaidya, V (Vaidya, V.); Gendron-Marsolais, ML (Gendron-Marsolais, M. -l.); Botteon, A (Botteon, A.); Roberts, ID (Roberts, I. D.); Hlavacek-Larrondo, J (Hlavacek-Larrondo, J.); Bonafede, A (Bonafede, A.); Brüggen, M (Brueggen, M.); Brunetti, G (Brunetti, G.); Cassano, R (Cassano, R.); Cuciti, V (Cuciti, V.); Edge, AC (Edge, A. C.); Gastaldello, F (Gastaldello, F.); Groeneveld, C (Groeneveld, C.); Shimwell, TW (Shimwell, T. W.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 692 **Article Number:** A12 **DOI:** 10.1051/0004-6361/202451618 **Published Date:** 2024 NOV 28

Abstract: The Perseus cluster is the brightest X-ray cluster in the sky and is known as a cool-core galaxy cluster. Being a very nearby cluster, it has been extensively studied. This has provided a comprehensive view of the physical processes that operate in the intracluster medium (ICM), including feedback from the active galactic nucleus (AGN) 3C 84 and measurements of ICM turbulence. Additionally, the Perseus cluster contains a central radio mini-halo. This diffuse radio source traces cosmic-ray electrons (re-)accelerated in situ in the ICM. Here, we report on LOFAR high-band antenna 120-168 MHz observations of the Perseus cluster that probe a range of four orders of magnitude in angular scales. In our 0.3 " (0.11 kpc) resolution image, we find that the northern extension of the 3C 84 lobe consists of several narrow 1.5-3 kpc parallel strands of emission. In addition, we detect steep-spectrum filaments associated with a previous outburst of the central AGN radio emission filling two known X-ray "ghost" cavities. At 7 " resolution (2.6 kpc), our images show a complex structured radio mini-halo, with several edges and filaments. At resolutions of 26 " (10 kpc) and 80 " (29 kpc), we discover diffuse radio emission with a 1.1 Mpc extent. We classify this emission as a giant radio halo, and its properties are distinct from the inner mini-halo. We also detect two diffuse sources at projected cluster centric radii of 0.7 and 1.0 Mpc. Finally, we observe a 0.9 Mpc trail of radio emission from the cluster member galaxy IC 310 that connects it to the giant radio halo. Together with other recent studies of relaxed clusters, our LOFAR observations indicate that cluster-wide radio emission could be (more) common in cool-core clusters. In the case of the Perseus cluster, a past off-axis merger event that preserved the cool core might have generated enough turbulence to produce an extended radio halo observable at low frequencies.

Accession Number: WOS:001367213400003

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ISSN: 0004-6361

eISSN: 1432-0746

Record 74 of 274

Title: Charge delocalization and global aromaticity in a partially fused 12-porphyrin nanoring

Author(s): Kopp, SM (Kopp, Sebastian M.); Gotfredsen, H (Gotfredsen, Henrik); Hergenhahn, J (Hergenhahn, Janko); Rodríguez-Rubio, A (Rodriguez-Rubio, Arnau); Deng, JR (Deng, Jie-Ren); Zhu, H (Zhu, He); Stawski, W (Stawski, Wojciech); Anderson, HL (Anderson, Harry L.)

Source: CHEM **Volume:** 10 **Issue:** 11 **DOI:** 10.1016/j.chempr.2024.06.034 **Early Access Date:** NOV 2024 **Published Date:** 2024 NOV 14

Abstract: Aromatic and antiaromatic ring currents can reveal global electronic delocalization around the circumference of pi-conjugated macrocycles, although these phenomena are poorly understood in large rings. Here, we present the template-directed synthesis of a fully pi-conjugated cyclic porphyrin 12-mer consisting of six beta,meso,beta-edge-fused porphyrin dimers connected by six butadiyne bridges. The lowest energy pi-pi & lowast; absorption band of this partially fused nanoring is shifted far into the NIR, confirming strong pi-conjugation around the circumference of the macrocycle. Investigation of the oxidized and reduced nanoring-template complex by H-1 and F-19 NMR spectroscopy demonstrates the presence of coherent global (anti)aromatic ring currents, consistent with DFT calculations. The stronger pi-conjugation enables global charge delocalization even at low levels of oxidation or reduction. These findings open new avenues for the engineering of cyclic molecular wires.

Accession Number: WOS:001360062700001

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Stawski, Wojciech	LUY-7638-2024	

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Record 75 of 274

Title: The LOFAR two metre sky survey data release 2: probabilistic spectral source classifications and faint radio source demographics

Author(s): Drake, AB (Drake, A. B.); Smith, DJB (Smith, D. J. B.); Hardcastle, MJ (Hardcastle, M. J.); Best, PN (Best, P. N.); Kondapally, R (Kondapally, R.); Arnaudova, M (Arnaudova, M., I); Das, S (Das, S.); Shenoy, S (Shenoy, S.); Duncan, KJ (Duncan, K. J.); Rottgering, HJA (Rottgering, H. J. A.); Tasse, C (Tasse, C.)

Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY **Volume:** 534 **Issue:** 2 **Pages:** 1107-1126 **DOI:** 10.1093/mnras/stae2117 **Published Date:** 2024 SEP 26

Abstract: We present an analysis of 152 355 radio sources identified in the second data release of the LOFAR Two Metre Sky Survey (LoTSS-DR2) with Sloan Digital Sky Survey (SDSS) spectroscopic redshifts in the range $0.00 \lt z \lt 0.57$. Using Monte Carlo simulations, we determine the reliability of each source exhibiting an excess in radio luminosity relative to that predicted from their H α emission, and, for a subset of 124 023 sources we combine this measurement with a full BPT analysis. Using these two independent diagnostics, we determine the reliability of each source hosting a supermassive black hole of high or low Eddington-scaled accretion rate, and combine the measurements

to determine the reliability of sources belonging to each of four physical classes of objects: star-forming galaxies (SFGs), radio-quiet active galactic nuclei (RQAGN), and high- or low-excitation radio galaxies (HERGs or emission-line LERGs). The result is a catalogue that enables user-defined samples of radio sources with a reliability threshold suited to their science goal, for example prioritizing purity or completeness. Here, we select high-confidence samples of radio sources (>90 per cent reliability) to report: 38 588 radio-excess AGNs in the LoTSS-DR2 sample (362 HERGs, and 12 648 emission-line LERGs), together with 38 729 SFGs, and 18 726 RQAGN. We validate these results through comparison to literature using independent emission-line measurements, and to widely adopted WISE photometric selection techniques. While our use of SDSS spectroscopy limits our current analysis to ~ 4 per cent of the LoTSS-DR2 catalogue, our method is directly applicable to data from the forthcoming WEAVE-LOFAR survey, which will obtain over a million spectra of 144 MHz selected sources.

Accession Number: WOS:001320536900008

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ISSN: 0035-8711

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Record 76 of 274

Title: Triptycene-Based Tripodal Molecular Platforms

Author(s): Bastien, G (Bastien, Guillaume); Severa, L (Severa, Lukas); Skuta, M (Skuta, Martin); Hurtado, CS (Hurtado, Carina Santos); Rybácek, J (Rybacek, Jiri); Solínová, V (Solinova, Veronika); Cisarová, I (Cisarova, Ivana); Kasicka, V (Kasicka, Vaclav); Kaleta, J (Kaleta, Jiri)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 30 **Issue:** 56 **DOI:** 10.1002/chem.202401889 **Early Access Date:** SEP 2024 **Published Date:** 2024 OCT 8

Abstract: Molecular platforms are essential components of various surface-mounted molecular devices. Here, we document the synthesis of two universal triptycene-based tripodal pedestals featuring terminal alkynes in the axial position. We showcase their versatility by incorporating them into the structures of diverse functional molecules such as unidirectional light-driven molecular motors, photoswitches, and Brownian molecular rotors using standard cross-coupling reactions. We also present their fundamental physical properties, including acidity constants, data from differential scanning calorimetry, and crystallographic analysis of two parent and five derived structures. Finally, and importantly, we demonstrate that the photochemical properties of selected photoswitch representatives remain uncompromised when fused with tripods.
Two universal triptycene-based tripodal pedestals featuring terminal alkynes in the axial position are presented. Their versatility is showcased by incorporating them into the structures of diverse functional molecules such as unidirectional light-driven molecular motors, photoswitches, and Brownian molecular rotors. image

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ISSN: 0947-6539
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Record 77 of 274

Title: Designing carbon dots for enhanced photo-catalysis: Challenges and opportunities

Author(s): Zdrazil, L (Zdrazil, Lukas); Cadranel, A (Cadranel, Alejandro); Medved, M (Medved, Miroslav); Otyepka, M (Otyepka, Michal); Zbor, R (Zbor, Radek); Guldi, DM (Guldi, Dirk M.)

Source: CHEM **Volume:** 10 **Issue:** 9 **Pages:** 2700-2723 **DOI:** 10.1016/j.chempr.2024.07.018 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 12

Abstract: Carbon dots (CDs) are a fascinating class of nanomaterials with a straightforward design by means of an organic chemistry toolbox and an unsurmountable potential in the field of artificial photosynthesis. The vast structural diversity of CDs and the complex photo-physics thereof impose, however, significant challenges on their full utilization. Gathering a profound understanding of the structure-activity relationship and precise identification of the photo-catalytically active sites within CDs is crucial. This review summarizes the current understanding of photo-catalytically active CD-based systems. First, we analyze the structural complexity of CDs in the context of hydrogen photo-production, addressing the different roles of CDs in photo-catalytic hydrogen evolution as photosensitizers, co-catalysts, and catalysts. Second, we present the most important aspects to be considered for the design of CDs-based photo-catalysts, focusing on the fine-tuning of optical properties and charge management and discussing the timescales of events in the photo-excited state. Both experimental and theoretical methods relevant to studying structurally complex CDs are outlined. Finally, we share our thoughts on the future opportunities in CD-based photo-catalysis.

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ISSN: 2451-9294

Record 78 of 274

Title: Multitemperature atomic ensemble: Nonequilibrium evolution after ultrafast electronic excitation

Author(s): Medvedev, N (Medvedev, Nikita); Volkov, AE (Volkov, Alexander E.)

Source: PHYSICAL REVIEW E **Volume:** 110 **Issue:** 2 **Article Number:** 024142 **DOI:** 10.1103/PhysRevE.110.024142 **Published Date:** 2024 AUG 30

Abstract: Ultrafast laser radiation or beams of fast charged particles primarily excite the electronic system of a solid driving the target transiently out of thermal equilibrium. Apart from the nonequilibrium between the electrons and atoms, each subsystem may be far from equilibrium. From first principles, we derive the definition of various atomic temperatures applicable to electronically excited ensembles. It is shown that the definition of the kinetic temperature of atoms in the momentum subspace is unaffected by the excitation of the electronic system. When the electronic temperature differs from the atomic one, an expression for the configurational atomic temperature is proposed, applicable to the electronic-temperature-dependent interatomic potentials (such as ab initio molecular dynamics simulations). We study how the configurational temperature behaves during nonthermal phase transition, triggered by the evolution of the interatomic potential due to the electronic excitation. It is revealed that upon the ultrafast irradiation, the atomic system of a solid exists temporarily in a multitemperature state: separate equilibria in the momentum and configurational subspaces. Complete equilibration between the various atomic temperatures takes place at longer timescales, forming the energy equipartition. Based on these results,

we propose a formulation of multitemperature heat transport equations.

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Record 79 of 274

Title: Surface structure of MOVPE-prepared As-modified Si(100) substrates

Author(s): Bohlemann, CY (Bohlemann, Chris Yannic); Flötotto, A (Floetotto, Aaron); Paszuk, A (Paszuk, Agnieszka); Nandy, M (Nandy, Manali); Grossmann, M (Grossmann, Max); Romanyuk, O (Romanyuk, Oleksandr); Hanke, KD (Hanke, Kai Daniel); Giess, A (Giess, Aaron); Kleinschmidt, P (Kleinschmidt, Peter); Runge, E (Runge, Erich); Hannappel, T (Hannappel, Thomas)

Source: APPLIED SURFACE SCIENCE **Volume:** 675 **Article Number:** 160879 **DOI:** 10.1016/j.apsusc.2024.160879 **Early Access Date:** AUG 2024 **Published Date:** 2024 NOV 30

Abstract: In the pursuit of high-efficiency tandem devices for solar energy conversion based on III-V-semiconductors, low-defect III-V nucleation on Si(100) substrates is essential. Here, hydrogen and arsenic are key ingredients in all growth processes with respect to industrially scalable metalorganic vapor phase epitaxy. Our study provides insight into Si(100) surface preparation for the initial stage of III-V nucleation. The samples investigated, prepared on substrates with different offcut angles, show single domain surfaces consisting of rows of preferentially buckled dimers. Low energy electron diffraction and reflection anisotropy spectroscopy confirm well-defined (1 x 2) / (2 x 1) majority domains. Fourier-transform infrared spectroscopy revealed hydrogen bonding to the surface dimers, while no impurities were found by XPS. Density functional theory calculations support the experimental results and reveal a novel surface motif of H-passivated Si-As mixed dimers.

Accession Number: WOS:001298042400001

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ISSN: 0169-4332

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Record 80 of 274

Title: On the suitability of dispersion models of varying degree of complexity for air quality assessment and urban planning

Author(s): Patiño, WR (Patino, William R.); Vlcek, O (Vlcek, Ondrej); Bauerová, P (Bauerova, Petra); Belda, M (Belda, Michal); Bures, M (Bures, Martin); Eben, K (Eben, Krystof); Fuka, V (Fuka, Vladimir); Geletic, J (Geletic, Jan); Jares, R (Jares, Radek); Karel, J (Karel, Jan); Keder, J (Keder, Josef); Krc, P (Krc, Pavel); Radovic, J (Radovic, Jelena); Reznicek, H (Reznicek, Hynek); Sindelarova, A (Sindelarova, Adriana); Resler, J (Resler, Jaroslav)

Source: BUILDING AND ENVIRONMENT **Volume:** 264 **Article Number:** 111892 **DOI:** 10.1016/j.buildenv.2024.111892 **Early Access Date:** AUG 2024 **Published Date:** 2024 OCT 1

Abstract: The development of integrated urban services requires the implementation of informative tools that provide a balance between quality, time and costs for air quality assessment. Within this framework, three modeling techniques with different levels of complexity were compared during a winter inversion episode against PM10 10 concentrations measured in a built-up area in Prague (Czech Republic) characterized by heavy traffic. Although the Gaussian model ATEM satisfied the common statistical-performance criteria, the predictions poorly represented the spatial variability of concentrations in the study domain. The Lagrangian model GRAL provided a better simulation of the effects of terrain and vortice formation inside street canyons, but tended to overpredict the influence of these phenomena. Finally, the most sophisticated of the three models, the Large-Eddy Simulation model PALM, demonstrated the best performance based on an exhaustive analysis of the model outputs in the temporal and spatial dimensions. After model comparison, a sensitivity test of the selected models to the driving meteorology and emissions inputs was carried out. While advanced models can simulate complex urban environments, their suitability for use in urban planning is subject to further considerations, such as computational cost, user expertise, and the usefulness of the output. Thanks to increasing computation power and intensive work on the entire modeling chain, sophisticated models could become routine tools for use in regulatory applications, contributing to future integrated urban service provision.

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Record 81 of 274

Title: Fractional positional jumps in stochastic systems with tilted periodic double-well potentials

Author(s): Zonda, M (Zonda, Martin); Belzig, W (Belzig, Wolfgang); Goldobin, E (Goldobin, Edward); Novotny, T (Novotny, Tomas)

Source: PHYSICAL REVIEW B **Volume:** 110 **Issue:** 5 **Article Number:** 054306 **DOI:** 10.1103/PhysRevB.110.054306 **Published Date:** 2024 AUG 7

Abstract: We present a theoretical investigation of the stochastic dynamics of a damped particle in a tilted periodic potential with a double well per period. By applying the matrix continued fraction technique to the Fokker-Planck equation in conjunction with the full counting statistics and master equation approaches, we determine the rates of specific processes contributing to the system's overall dynamics. At low temperatures, the system can exhibit one running state and two distinct locked metastable states. We focus primarily on two aspects: the dynamics of positional jumps, which are rare thermally induced particle jumps over potential maxima, and their impact on the overall velocity noise;

and the retrapping process, involving the transition from the running to the locked metastable states. We demonstrate the existence of fractional (in units of 2 pi) positional slips that differ qualitatively from conventional 2 pi jumps observed in single-well systems. Fractional positional slips significantly influence the system dynamics even in regimes dominated by dichotomous-like switching between running and locked states. Furthermore, we introduce a simple master equation approach that proves effective in analyzing various stages of the retrapping process. Interestingly, our analysis shows that even for a system featuring a well-developed double-well periodic potential, there exists a broad parameter range where the stochastic dynamics can be accurately described by an effective single-well periodic model. The techniques introduced here allow for valuable insights into the complex behavior of the system, offering avenues for understanding and controlling its steady-state and transient dynamics, which go beyond or can be complementary to direct stochastic simulations.

Accession Number: WOS:001290016400002

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ISSN: 2469-9950

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Record 82 of 274

Title: Variation in induced responses in volatile and non-volatile metabolites among six willow species: Do willow species share responses to herbivory?

Author(s): Mezzomo, P (Mezzomo, Priscila); Leong, JV (Leong, Jing V.); Vodrazka, P (Vodrazka, Petr); Moos, M (Moos, Martin); Jorge, LR (Jorge, Leonardo R.); Volfová, T (Volfova, Tereza); Michálek, J (Michalek, Jan); Ferreira, PD (Ferreira, Paola de L.); Kozel, P (Kozel, Petr); Sedio, BE (Sedio, Brian E.); Volf, M (Volf, Martin)

Source: PHYTOCHEMISTRY **Volume:** 226 **Article Number:** 114222 **DOI:** 10.1016/j.phytochem.2024.114222 **Early Access Date:** JUL 2024 **Published Date:** 2024 OCT

Abstract: Chemical variation is a critical aspect affecting performance among co-occurring plants. High chemical variation in metabolites with direct effects on insect herbivores supports chemical niche partitioning, and it can reduce the number of herbivores shared by co-occurring plant species. In contrast, low intraspecific variation in metabolites with indirect effects, such as induced volatile organic compounds (VOCs), may improve the attraction of specialist predators or parasitoids as they show high specificity to insect herbivores. We explored whether induced chemical variation following herbivory by various insect herbivores differs between VOCs vs. secondary non-volatile metabolites (non-VOCs) and salicinoids with direct effects on herbivores in six closely related willow species. Willow species identity explained most variation in VOCs (18.4%), secondary non-VOCs (41.1%) and salicinoids (60.7%). The variation explained by the independent effect of the herbivore treatment was higher in VOCs (2.8%) compared to secondary non-VOCs (0.5%) and salicinoids (0.5%). At the level of individual VOCs, willow species formed groups, as some responded similarly to the same herbivores. Most non-VOCs and salicinoids were upregulated by sap-suckers compared to other herbivore treatments and control across the willow species. In contrast, induced responses in non-VOCs and salicinoids to other herbivores largely differed between the willows. Our results suggest that induced responses broadly differ between various types of chemical defences, with VOCs and non-VOCs showing different levels of specificity and similarity across plant species. This may further contribute to flexible plant responses to herbivory and affect how closely related plants share or partition their chemical niches.

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PubMed ID: 39047854

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Record 83 of 274

Title: Caenorhabditis elegans SEL-5/AAK1 regulates cell migration and cell outgrowth independently of its kinase activity

Author(s): Knop, F (Knop, Filip); Zounarová, A (Zounarova, Apolena); Sabata, V (Sabata, Vojtech); Middelkoop, TC (Middelkoop, Teije Corneel); Macurková, M (Macurkova, Marie)

Source: ELIFE **Volume:** 13 **Article Number:** e91054 **DOI:** 10.7554/eLife.91054 **Published Date:** 2024 JUL 19

Abstract: During Caenorhabditis elegans development, multiple cells migrate long distances or extend processes to reach their final position and/or attain proper shape. The Wnt signalling pathway stands out as one of the major coordinators of cell migration or cell outgrowth along the anterior-posterior body axis. The outcome of Wnt signalling is fine-tuned by various mechanisms including endocytosis. In this study, we show that SEL-5, the C. elegans orthologue of mammalian AP2-associated kinase AAK1, acts together with the retromer complex as a positive regulator of EGL-20/Wnt signalling during the migration of QL neuroblast daughter cells. At the same time, SEL-5 in cooperation with the retromer complex is also required during excretory canal cell outgrowth. Importantly, SEL-5 kinase activity is not required for its role in neuronal migration or excretory cell outgrowth, and neither of these processes is dependent on DPY-23/AP2M1 phosphorylation. We further establish that the Wnt proteins CWN-1 and CWN-2, together with the Frizzled receptor CFZ-2, positively regulate excretory cell outgrowth, while LIN-44/Wnt and LIN-17/Frizzled together generate a stop signal inhibiting its extension.

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PubMed ID: 39028260

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ISSN: 2050-084X

Record 84 of 274

Title: Fibrotic extracellular matrix impacts cardiomyocyte phenotype and function in an iPSC-derived isogenic model of cardiac fibrosis

Author(s): Niro, F (Niro, Francesco); Fernandes, S (Fernandes, Soraia); Cassani, M (Cassani, Marco); Apostolico, M (Apostolico, Monica); de la Cruz, J (de la Cruz, Jorge); Pereira-Sousa, D (Pereira-Sousa, Daniel); Pagliari, S (Pagliari, Stefania); Vinarsky, V (Vinarsky, Vladimir); Zdrahal, Z (Zdrahal, Zbynek); Potesil, D (Potesil, David); Pustka, V (Pustka, Vaclav); Pompilio, G (Pompilio, Giulio); Sommariva, E (Sommariva, Elena); Rovina, D (Rovina, Davide); Maione, AS (Maione, Angela Serena); Bersanini, L (Bersanini, Luca); Becker, M (Becker, Malin); Rasponi, M (Rasponi, Marco); Forte, G (Forte, Giancarlo)

Source: TRANSLATIONAL RESEARCH **Volume:** 273 **Pages:** 58-77 **DOI:** 10.1016/j.trsl.2024.07.003 **Early Access Date:** JUL 2024 **Published Date:** 2024 NOV

Abstract: Cardiac fibrosis occurs following insults to the myocardium and is characterized by the abnormal accumulation of non-compliant extracellular matrix (ECM), which compromises cardiomyocyte contractile activity and eventually leads to heart failure. This phenomenon is driven by the activation of cardiac fibroblasts (cFbs) to myofibroblasts and results in changes in ECM biochemical, structural and mechanical properties. The lack of predictive in vitro models of heart fibrosis has so far hampered the search for innovative treatments, as most of the cellular-based in vitro reductionist models do not take into account the leading role of ECM cues in driving the progression of the pathology. Here, we devised a single-step decellularization protocol to obtain and thoroughly characterize the biochemical and micro-mechanical properties of the ECM secreted by activated cFbs differentiated from human induced pluripotent stem cells (iPSCs). We activated iPSC-derived cFbs to the myofibroblast phenotype by tuning basic fibroblast growth factor (bFGF) and transforming growth factor beta 1 (TGF-beta 1) signalling and confirmed that activated cells acquired key features of myofibroblast phenotype, like SMAD2/3 nuclear shuttling, the formation of aligned alpha-smooth muscle actin (alpha- SMA)-rich stress fibres and increased focal adhesions (FAs) assembly. Next, we used Mass Spectrometry, nanoindentation, scanning electron and confocal microscopy to unveil the characteristic composition and the visco-elastic properties of the abundant, collagen-rich ECM deposited by cardiac myofibroblasts in vitro. Finally, we demonstrated that the fibrotic ECM activates mechanosensitive pathways in iPSC-derived cardiomyocytes, impacting on their shape, sarcomere assembly, phenotype, and calcium handling properties. We thus propose human bio-inspired decellularized matrices as animal-free, isogenic cardiomyocyte culture substrates recapitulating key pathophysiological changes occurring at the cellular level during cardiac fibrosis.

Accession Number: WOS:001275554600001

PubMed ID: 39025226

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ISSN: 1931-5244

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Record 85 of 274

Title: Single-atom catalysis in space: II. Ketene-acetaldehyde-ethanol and methane synthesis via Fischer-Tropsch chain growth

Author(s): Pareras, G (Pareras, G.); Cabedo, V (Cabedo, V.); Mccoustra, M (Mccoustra, M.); Rimola, A (Rimola, A.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 687 **Article Number:** A230 **DOI:** 10.1051/0004-6361/202449378 **Published Date:** 2024 JUL 18

Abstract: Context. The presence of grains is key to the synthesis of molecules in the interstellar medium that cannot form in the gas phase due to its low density and temperature conditions. In these reactions, the role of the grains is to enhance the encounter rate of the reactive species on their surfaces and to dissipate the energy excess of largely exothermic reactions, but less is known about their role as chemical catalysts; namely, bodies that provide low activation energy pathways with enhanced reaction rates. Different refractory materials with catalytic properties, such as those containing space-abundant d-block transition metals like iron (Fe), are present in astrophysical environments. Aims. Here, we report for first time mechanistic insights into the Fischer-Tropsch-type (FTT) synthesis of ethanol (CH3CH2OH), through ketene (CH2CO) and acetaldehyde (CH3CHO) intermediates, and methane (CH4) via a chain growing mechanism using a single-Fe atom supported on silica (SiO2) surfaces as a heterogeneous astrocatalyst. Methods. Quantum chemical simulations based on extended periodic surfaces were carried out to characterize the potential energy surfaces of the FTT chain growing mechanism. Calculations of the binding energies of reaction intermediates and products and Rice-Ramsperger-Kassel-Marcus kinetic calculations were performed to evaluate catalytic efficiencies and determine the feasibility of the reactions in different astrophysical environments. Results. Mechanistic studies demonstrate that the FTT chain growing mechanism enters into direct competition with FTT methanol formation, since formation of the CH2 chain growth initiator is feasible. The coupling of the CH2 with CO (forming ketene) and subsequent H-2 additions yield acetaldehyde and finally ethanol, while direct H-2 addition to CH2 produces methane. Thermodynamically, both processes are largely exergonic, but they present energy barriers that require external energy inputs to be overcome. Kinetic calculations demonstrate the strong temperature dependency of the FTT processes as tunneling does not dominate. Conclusions. The results could explain the presence of CH3CH2OH and CH4 in diverse astrophysical regions where current models fail to reproduce their observational quantities. The evidence that the chain growing mechanism is operating opens a new reactivity paradigm toward the formation of complex organic molecules, which is constrained by the temperature-dependent behaviour of the FTT reactions and by making their energy features a crucial aspect.

Accession Number: WOS:001272897700001

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eISSN: 1432-0746

Record 86 of 274

Title: Protonation of palmitic acid embedded in DPPC lipid bilayers obscures detection of ripple phase by FTIR spectroscopy

Author(s): Pem, B (Pem, Barbara); Pisonic, M (Pisonic, Marina); Momcilov, M (Momcilov, Marina); Crnolatac, I (Crnolatac, Ivo); Brkljaca, Z (Brkljaca, Zlatko); Vazdar, M (Vazdar, Mario); Bakaric, D (Bakaric, Danijela)

Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 322 **Article Number:** 124773 **DOI:** 10.1016/j.saa.2024.124773 **Early Access Date:** JUL 2024 **Published Date:** 2024 DEC 5

Abstract: The transformation of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) lipid bilayers from the gel (L beta ') to the fluid (L alpha) phase involves an intermediate ripple (P beta ') phase forming a few degrees below the main transition temperature (Tm). While the exact cause of bilayer

rippling is still debated, the presence of amphiphilic molecules, pH, and lipid bilayer architecture are all known to influence (pre)transition behavior. In particular, fatty acid chains interact with hydrophobic lipid tails, while the carboxylic groups simultaneously participate in proton transfer with interfacial water in the polar lipid region which is controlled by the pH of the surrounding aqueous medium. The molecular-level variations in the DPPC ripple phase in the presence of 2% palmitic acid (PA) were studied at pH levels 4.0, 7.3, and 9.1, where PA is fully protonated, partially protonated, or fully deprotonated. Bilayer thermotropic behavior was investigated by differential scanning calorimetry (DSC) and Fourier-transform infrared (FTIR) spectroscopy which agreed in their characterization of (pre)transition at pH of 9.1, but not at pH 4.0 and especially not at 7.3. Owing to the different insertion depths of protonated and deprotonated PA, along with the ability of protonated PA to undergo flip-flop in the bilayer, these two forms of PA show a different hydration pattern in the interfacial water layer. Finally, these results demonstrated the hitherto undiscovered potential of FTIR spectroscopy in the detection of the events occurring at the surface of lipid bilayers that obscure the low-cooperativity phase transition explored in this work.

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PubMed ID: 39002469

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ISSN: 1386-1425

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Record 87 of 274

Title: Histone Chaperone Deficiency in Arabidopsis Plants Triggers Adaptive Epigenetic Changes in Histone Variants and Modifications

Author(s): Franek, M (Franek, Michal); Dadejová, MN (Dadejova, Martina Nespor); Pírek, P (Pirek, Pavlina); Krystofová, K (Krystofova, Karolina); Dobisová, T (Dobisova, Tereza); Zdráhal, Z (Zdrahal, Zbynek); Dvoárková, M (Dvoarkova, Martina); Lochmanová, G (Lochmanova, Gabriela)

Source: MOLECULAR & CELLULAR PROTEOMICS **Volume:** 23 **Issue:** 7 **Article Number:** 100795 **DOI:** 10.1016/j.mcpro.2024.100795 **Published Date:** 2024 JUL

Abstract: At the molecular scale, adaptive advantages during plant growth and development rely on modulation of gene expression, primarily provided by epigenetic machinery. One crucial part of this machinery is histone post- translational modifications, which form a flexible system, driving transient changes in chromatin, and defining particular epigenetic states. Posttranslational modifications work in concert with replication-independent histone variants further adapted for transcriptional regulation and chromatin repair. However, little is known about how such complex regulatory pathways are orchestrated and interconnected in cells. In this work, we demonstrate the utility of mass spectrometry-based approaches to explore how different epigenetic layers interact in Arabidopsis mutants lacking certain histone chaperones. We show that defects in histone chaperone function (e.g. , chromatin assembly factor-1 or nucleosome assembly protein 1 mutations) translate into an altered epigenetic landscape, which aids the plant in mitigating internal instability. We observe changes in both the levels and distribution of H2A.W.7, altogether with partial repurposing of H3.3 and changes in the key repressive (H3K27me1/2) or euchromatic marks (H3K36me1/2). These shifts in the epigenetic profile serve as a compensatory mechanism in response to impaired integration of the H3.1 histone in the fas1 mutants. Altogether, our findings suggest that maintaining genome stability involves a two-tiered approach. The first relies on flexible adjustments in histone marks, while the second level requires the assistance of

chaperones for histone variant replacement.

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PubMed ID: 38848995

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eISSN: 1535-9484

Record 88 of 274

Title: Extensive targeting of chemical space at the prime side of ketoamide inhibitors of rhomboid proteases by branched substituents empowers their selectivity and potency

Author(s): Bach, K (Bach, Kathrin); Dohnálek, J (Dohnalek, Jan); Skerlová, J (Skerlova, Jana); Kuzmík, J (Kuzmik, Jan); Poláchová, E (Polachova, Edita); Stanchev, S (Stanchev, Stancho); Majer, P (Majer, Pavel); Fanfrlík, J (Fanfrlik, Jindich); Pecina, A (Pecina, Adam); Rezác, J (Rezac, Jan); Lepsík, M (Lepsik, Martin); Borshchevskiy, V (Borshchevskiy, Valentin); Polovinkin, V (Polovinkin, Vitaly); Strisovsky, K (Strisovsky, Kvido)

Source: EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY **Volume:** 275 **Article Number:** 116606 **DOI:** 10.1016/j.ejmech.2024.116606 **Early Access Date:** JUN 2024 **Published Date:** 2024 SEP 5

Abstract: Rhomboid intramembrane serine proteases have been implicated in several pathologies, and emerge as attractive pharmacological target candidates. The most potent and selective rhomboid inhibitors available to date are peptidyl alpha-ketoamides, but their selectivity for diverse rhomboid proteases and strategies to modulate it in relevant contexts are poorly understood. This gap, together with the lack of suitable in vitro models, hinders ketoamide development for relevant eukaryotic rhomboid enzymes. Here we explore the structure-activity relationship principles of rhomboid inhibiting ketoamides by medicinal chemistry and enzymatic in vitro and in-cell assays with recombinant rhomboid proteases GlpG, human mitochondrial rhomboid PARL and human RHBDL2. We use X-ray crystallography in lipidic cubic phase to understand the binding mode of one of the best ketoamide inhibitors synthesized here containing a branched terminal substituent bound to GlpG. In addition, to extend the interpretation of the co-crystal structure, we use quantum mechanical calculations and quantify the relative importance of interactions along the inhibitor molecule. These combined experimental analyses implicates that more extensive exploration of chemical space at the prime side is unexpectedly powerful for the selectivity of rhomboid inhibiting ketoamides. Together with variations in the peptide sequence at the non-prime side, or its non-peptidic alternatives, this strategy enables targeted tailoring of potent and selective ketoamides towards diverse rhomboid proteases including disease-relevant ones such as PARL and RHBDL2.

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PubMed ID: 38901105

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Record 89 of 274

Title: Facile synthesis and bonding of 4-ferrocenyl-1,2,4-triazol-5-ylidene complexes

Author(s): Franc, M (Franc, Michal); Schulz, J (Schulz, Jiri); Stepnicka, P (Stepnicka, Petr)

Source: DALTON TRANSACTIONS **Volume:** 53 **Issue:** 27 **Pages:** 11445-11453 **DOI:** 10.1039/d4dt01433b **Early Access Date:** JUN 2024 **Published Date:** 2024 JUL 9

Abstract: Ferrocene-substituted carbenes have emerged as attractive, redox-active ligands. However, among the compounds studied to date, ferrocenylated 1,2,4-triazol-5-ylidenes, which are closely related to the archetypal imidazol-2-ylidenes, are still unknown. Here, we demonstrate that the triazolium salt [CHN(Me)NCHN(Fc)]I (2; Fc = ferrocenyl), obtained by alkylation of 4-ferrocenyl-4H-1,2,4-triazole (1) with MeI, reacts selectively with metal alkoxide/hydroxide precursors [(cod)Rh(OMe)]2 and [(IPr)Au(OH)] (cod = cycloocta-1,5-diene, IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene) to produce the ferrocene-substituted 1,2,4-triazol-5-ylidene complexes [(cod)RhI{CN(Me)NCHN(Fc)}] and [(IPr)Au{CN(Me)NCHN(Fc)}]I in good yields. The complexes were characterised by NMR and IR spectroscopy, mass spectrometry, cyclic voltammetry, and single-crystal X-ray diffraction analysis. Density function theory (DFT) calculations were used to rationalise the electrochemical behaviour of the carbene complexes and to elucidate the bonding situation in these compounds. An analysis using intrinsic bond orbitals (IBOs) revealed that the 1,2,4-triazol-5-ylidene ligand exerted a strong trans influence and showed a synergistic stabilisation by the negative inductive and positive pi-donor effects of the nitrogen atoms adjacent to the carbene carbon atom; these effects were enhanced by conjugation with the CH 00000000 00000000 00000000 00000000 11111111 00000000 11111111 00000000 00000000 00000000 N bond at the exterior, similar to that in imidazol-2-ylidenes.
Triazolium salt obtained by alkylation of 4-ferrocenyl-4H-1,2,4-triazole reacts smoothly with metal hydroxides and alkoxides to produce 4-ferrocenyl-1,2,4-triazol-5-ylidene complexes, whose bonding was studied experimentally and theoretically.

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PubMed ID: 38904982

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Record 90 of 274

Title: Role of Cyclodextrin Cross-Linker Type on Steroid Hormone Micropollutant Removal from Water Using Composite Nanofiber Membrane

Author(s): Lin, HY (Lin, Han Ya); Imbrogno, A (Imbrogno, Alessandra); Gopalakrishnan, A (Gopalakrishnan, Akhil); Minofar, B (Minofar, Babak); Schäfer, AI (Schaefer, Andrea I.)

Source: ACS APPLIED POLYMER MATERIALS **Volume:** 6 **Issue:** 12 **Pages:** 7184-7196 **DOI:** 10.1021/acsapm.4c01019 **Early Access Date:** JUN 2024 **Published Date:** 2024 JUN 18

Abstract: Cross-linkers employed to enhance cyclodextrin's (CD) stability and mechanical strength in composite polymers may additionally enhance micropollutant removal. The impact of cross-linker types on the interaction, removal, and uptake of steroid hormones (SHs) with cross-linked beta-cyclodextrin polymer (beta CDP) in functionalized composite nanofiber membranes (CNMs) was investigated. The

primary objective of the study was to assess the efficiency of CNM cross-linking with triphenylolmethane triglycidyl ether (TMTE) and trimethylolpropane triglycidyl ether (TPTE) in eliminating SH, as compared to the extensively used epichlorohydrin (EP) that is recognized for its higher toxicity and epoxy-based structure. Fourier-transform infrared spectroscopy (FTIR) confirmed the formation of the cross-linked beta CDP structure, while thermogravimetric analysis (TGA) validated the successful immobilization of beta CDP in nanofiber matrix membranes before and after filtration. The type of cross-linker influenced the uptake of SHs and their removal by the beta CD molecules during filtration. The highest SH removal was achieved with beta CD-EP and beta CD-TPTE, reaching 67 +/- 4 and 59 +/- 5%, with respective uptake values of 10.6 and 9.7 ng/cm2 at a flux of 600 L/m2h and using the nanofiber matrix thickness of 320 and 528 mu m. beta CD-TMTE exhibited the lowest removal (22 +/- 7%) and uptake (4.9 ng/cm2) due to the hindrance posed by its Y-shaped polymeric chain, which limited access to the beta CD cavity. Molecular dynamics simulations further supported these experimental findings, illustrating a more dispersed spatial distribution of SH molecules around the beta CD cavity when TPTE and TMTE were used as cross-linkers, in contrast to EP. In conclusion, triphenylphosphine glycidyl ether (TPTE) could be used as a potential alternative for EP in beta CDP CNMs, given the comparable efficacy in SH removal and uptake. This study highlights the significance of cross-linker selection for designing cyclodextrin-based materials applied to micropollutant removal from water.

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Record 91 of 274

Title: Direct laser acceleration: A model for the electron injection from the walls of a cylindrical guiding structure

Author(s): Valenta, P (Valenta, P.); Maslarova, D (Maslarova, D.); Babjak, R (Babjak, R.); Martinez, B (Martinez, B.); Bulanov, SV (Bulanov, S. V.); Vranic, M (Vranic, M.)

Source: PHYSICAL REVIEW E **Volume:** 109 **Issue:** 6 **Article Number:** 065204 **DOI:** 10.1103/PhysRevE.109.065204 **Published Date:** 2024 JUN 5

Abstract: We use analytical methods and particle -in -cell simulation to investigate the origin of electrons accelerated by the process of direct laser acceleration driven by high -power laser pulses in preformed narrow cylindrical plasma channels. The simulation shows that the majority of accelerated electrons are originally located along the interface between the channel wall and the channel interior. The analytical model based on the electron hydrodynamics illustrates the underlying physical mechanism of the release of electrons from the channel wall when irradiated by an intense laser, the subsequent electron dynamics, and the corresponding evolution of the channel density profile. The quantitative predictions of the total charge of released electrons and the average electron density inside the channel are validated by comparison with the simulation results.

Accession Number: WOS:001241449800005

PubMed ID: 39020949

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ISSN: 2470-0045

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Record 92 of 274

Title: Vibrational circular dichroism of adenosine crystals

Author(s): Krupová, M (Krupova, Monika); Leszczenko, P (Leszczenko, Patrycja); Sierka, E (Sierka, Ewa); Hamplova, SE (Hamplova, Sara Emma); Klepetárová, B (Klepetarova, Blanka); Pelc, R (Pelc, Radek); Andrushchenko, V (Andrushchenko, Valery)

Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 319 **Article Number:** 124381 **DOI:** 10.1016/j.saa.2024.124381 **Early Access Date:** JUN 2024 **Published Date:** 2024 OCT 15

Abstract: Adenosine is one of the building blocks of nucleic acids and other biologically important molecules. Spectroscopic methods have been among the most utilized techniques to study adenosine and its derivatives. However, most of them deal with adenosine in solution. Here, we present the first vibrational circular dichroism (VCD) spectroscopic study of adenosine crystals in solid state. Highly regular arrangement of adenosine molecules in a crystal resulted in a strongly enhanced supramolecular VCD signal originating from long-range coupling of vibrations. The data suggested that adenosine crystals, in contrast to guanosine ones, do not imbibe atmospheric water. Relatively large dimensions of the adenosine crystals resulted in scattering and substantial orientational artifacts affecting the spectra. Several strategies for tackling the artifacts have been proposed and tested. Atypical features in IR absorption spectra of crystalline adenosine (e.g., extremely low absorption in mid-IR spectral range) were observed and attributed to refractive properties of adenosine crystals.

Accession Number: WOS:001263636300001

PubMed ID: 38838602

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Andrushchenko, Valery	G-7970-2014	0000-0002-4874-0548

ISSN: 1386-1425

eISSN: 1873-3557

Record 93 of 274

Title: A machine learning approach for dynamical modelling of Al distributions in zeolites via²³Na/²⁷Al solid-state NMR

Author(s): Lei, C (Lei, Chen); Bornes, C (Bornes, Carlos); Bengtsson, O (Bengtsson, Oscar); Erlebach, A (Erlebach, Andreas); Slater, B (Slater, Ben); Grajciar, L (Grajciar, Lukas); Heard, CJ (Heard, Christopher J.)

Source: FARADAY DISCUSSIONS **Volume:** 255 **Issue:** 0 **DOI:** 10.1039/d4fd00100a **Early Access Date:** JUN 2024 **Published Date:** 2025 JAN 8

Abstract: One of the main limitations in supporting experimental characterization of Al siting/pairing via modelling is the high computational cost of ab initio calculations. For this reason, most works rely on static or very short dynamical simulations, considering limited Al pairing/siting combinations. As a

result, comparison with experiment suffers from a large degree of uncertainty. To alleviate this limitation we have developed neural network potentials (NNPs) which can dynamically sample across broad configurational and chemical spaces of sodium-form aluminosilicate zeolites, preserving the level of accuracy of the ab initio (dispersion-corrected metaGGA) training set. By exploring a wide range of Al/Na arrangements and a combination of experimentally relevant Si/Al ratios, we found that the Na-23 NMR spectra of dehydrated high-silica CHA zeolite offer an opportunity to assess the distribution and pairing of Al atoms. We observed that the Na-23 chemical shift is sensitive not only to the location of sodium in 6- and 8MRs, but also to the Al-Si-n-Al sequence length. Furthermore, neglect of thermal and dynamical contributions was found to lead to errors of several ppm, and has a profound influence on the shape of the spectra and the dipolar coupling constants, thus necessitating the long-term dynamical simulations made feasible by NNPs. Finally, we obtained a predictive regression model for the Na-23 chemical shift in CHA (Si/Al = 35, 17, 11) that circumvents the need for expensive NMR density functional calculations and can be easily extended to other zeolite frameworks. By combining NNPs and regression methods, we can expedite the simulations of NMR properties and capture the effect of dynamics on the spectra, which is often overlooked in computational studies despite its clear manifestation in experimental setups.

Accession Number: WOS:001331539100001

PubMed ID: 39382089

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Lei, Chen		0000-0002-0373-7433

ISSN: 1359-6640

eISSN: 1364-5498

Record 94 of 274

Title: Giant radio galaxies in the LOFAR deep fields

Author(s): Simonte, M (Simonte, M.); Andernach, H (Andernach, H.); Brueggen, M (Brueggen, M.); Miley, GK (Miley, G. K.); Barthel, P (Barthel, P.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 686 **Article Number:** A21 **DOI:** 10.1051/0004-6361/202348904 **Published Date:** 2024 MAY 27

Abstract: Context. The reason why some radio galaxies (RGs) grow to form so-called giant radio galaxies (GRGs) with sizes > 700 kpc, is still unknown. Aims. In this study, we compare the radio, optical and environmental properties of GRGs with those of a control sample of smaller RGs we found in the three LOw-Frequency ARray (LOFAR) deep fields, namely the Bo ötes, ELAIS-N1, Lockman Hole, for a total area of approximate to 95 deg2. Methods. We inspected the LOFAR deep fields and created a catalogue of 1609 extended radio galaxies (ERGs). By visual inspection, we identified their host galaxies and spectroscopically or photometrically classified 280 of these as GRGs. We studied their properties, such as their accretion state, stellar mass and star formation rate (SFR) using deep optical and infrared survey data. Moreover, we explored the environment in terms of the surface number density of neighbouring galaxies within these surveys. Integrated flux densities and radio luminosities were also determined for a subset of ERGs through available survey images at 50, 150, 610, and 1400 MHz to compute integrated spectral indices. Results. Considering the fraction of GRGs displaying an FRII morphology alongside the host galaxy properties, we suggest that GRGs consistently possess sufficient power to overcome jet frustration caused by the interstellar medium. Moreover, clear differences emerge in the environmental densities between GRGs and smaller RGs, using the number of neighbouring

galaxies within 10 Mpc from the host galaxy as a proxy. GRGs preferentially reside in sparser environments compared to their smaller counterparts. In particular, only 3.6% of the GRGs reside within a 3D comoving distance of 5 Mpc from a previously reported galaxy cluster. We found that larger sources exhibit steeper integrated spectral indices, suggesting that GRGs are late-stage versions of RGs. These results suggest that GRGs are amongst the oldest radio sources with the most stable nuclear activity that reside in sparse environments.

Accession Number: WOS:001231909000002

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ISSN: 0004-6361

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Record 95 of 274

Title: Solid-state vibrational circular dichroism for pharmaceutical applications: Polymorphs and cocrystal of sofosbuvir

Author(s): Sklenár, A (Sklenar, Adam); Ruzicková, L (Ruzickova, Lucie); Schrenková, V (Schrenkova, Vera); Bednárová, L (Bednarova, Lucie); Pazderková, M (Pazderkova, Marketa); Chatziadi, A (Chatziadi, Argyro); Skorepová, EZ (Skorepova, Eliska Zmeskalova); Soós, M (Soos, Miroslav); Kaminsky, J (Kaminsky, Jakub)

Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 318 **Article Number:** 124478 **DOI:** 10.1016/j.saa.2024.124478 **Early Access Date:** MAY 2024 **Published Date:** 2024 OCT 5

Abstract: X-ray diffraction is a commonly used technique in the pharmaceutical industry for the determination of the atomic and molecular structure of crystals. However, it is costly, sometimes time-consuming, and it requires a considerable degree of expertise. Vibrational circular dichroism (VCD) spectroscopy resolves these limitations, while also exhibiting substantial sensitivity to subtle modifications in the conformation and molecular packaging in the solid state. This study showcases VCD ' s ability to differentiate between various crystal structures of the same molecule (polymorphs, cocrystals). We examined the most effective approach for producing high -quality spectra and unveiled the intricate link between structure and spectrum via quantum -chemical computations. We rigorously assessed, using alanine as a model compound, multiple experimental conditions on the resulting VCD spectra, with the aim of proposing an optimal and efficient procedure. The proposed approach, which yields reliable, reproducible, and artifact -free results with maximal signal-to-noise ratio, was then validated using a set comprising of three amino acids (serine, alanine, tyrosine), one hydroxy acid (tartaric acid), and a monosaccharide (ribose) to mimic active pharmaceutical components. Finally, the optimized approach was applied to distinguish three polymorphs of the antiviral drug sofosbuvir and its cocrystal with piperazine. Our results indicate that solid-state VCD is a prompt, cost-effective, and easy -to -use technique to identify crystal structures, demonstrating potential for application in pharmaceuticals. We also adapted the cluster and transfer approach to calculate the spectral properties of molecules in a periodic crystal environment. Our findings demonstrate that this approach reliably produces solid-state VCD spectra of model compounds. Although for large molecules with many atoms per unit cell, such as sofosbuvir, this approach has to be simplified and provides only a qualitative match, spectral calculations, and energy analysis helped us to decipher the observed differences in the experimental spectra of sofosbuvir.

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PubMed ID: 38788502

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Record 96 of 274

Title: Diaminocyclopentane - L-Lysine Adducts: Potent and selective inhibitors of human O-GlcNAcase

Author(s): Weber, P (Weber, Patrick); Bojarová, P (Bojarova, Pavla); Brouzdová, J (Brouzdova, Jitka); Kulik, N (Kulik, Natalia); Stütz, AE (Stuetz, Arnold E.); Thonhofer, M (Thonhofer, Martin); Wrodnigg, TM (Wrodnigg, Tanja M.)

Source: BIOORGANIC CHEMISTRY **Volume:** 148 **Article Number:** 107452 **DOI:** 10.1016/j.bioorg.2024.107452 **Early Access Date:** MAY 2024 **Published Date:** 2024 JUL

Abstract: A new class of compounds, namely highly substituted diaminocyclopentane-L-lysine adducts, have been discovered as potent inhibitors of O-GlcNAcase, an enzyme crucial for protein de-O-glycosylation. These inhibitors exhibit exceptional selectivity and reversibility and are the first example of human O-GlcNAcase inhibitors that are structurally related to the transition state of the rate-limiting step with the "aglycon" still in bond-length proximity. The ease of their preparation, remarkable biological activities, stability, and nontoxicity make them promising candidates for the development of anti-tau-phosphorylation agents holding significant potential for the treatment of Alzheimer's disease.

Accession Number: WOS:001243022500001

PubMed ID: 38763001

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ISSN: 0045-2068

eISSN: 1090-2120

Record 97 of 274

Title: AlphaFind: discover structure similarity across the proteome in AlphaFold DB

Author(s): Procházka, D (Prochazka, David); Slanináková, T (Slaninakova, Terezia); Olha, J (Olha, Jaroslav); Rosinec, A (Rosinec, Adrian); Gresová, K (Gresova, Katarina); Jánosová, M (Janosova, Miriama); Cillík, J (Cillik, Jakub); Porubská, J (Porubska, Jana); Svobodová, R (Svobodova, Radka); Dohnal, V (Dohnal, Vlastislav); Antol, M (Antol, Matej)

Source: NUCLEIC ACIDS RESEARCH **Volume:** 52 **Issue:** W1 **Pages:** W182-W186 **DOI:** 10.1093/nar/gkae397 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 15

Abstract: AlphaFind is a web-based search engine that provides fast structure-based retrieval in the entire set of AlphaFold DB structures. Unlike other protein processing tools, AlphaFind is focused entirely on tertiary structure, automatically extracting the main 3D features of each protein chain and using a machine learning model to find the most similar structures. This indexing approach and the 3D feature extraction method used by AlphaFind have both demonstrated remarkable scalability to large datasets as well as to large protein structures. The web application itself has been designed with a focus on clarity and ease of use. The searcher accepts any valid UniProt ID, Protein Data Bank ID or gene symbol as input, and returns a set of similar protein chains from AlphaFold DB, including various similarity metrics between the query and each of the retrieved results. In addition to the main search functionality, the application provides 3D visualizations of protein structure superpositions in order to allow researchers to instantly analyze the structural similarity of the retrieved results. The AlphaFind web application is available online for free and without any registration at https://alphafind.fi.muni.cz. Graphical Abstract

Accession Number: WOS:001222684000001

PubMed ID: 38747341

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ISSN: 0305-1048

eISSN: 1362-4962

Record 98 of 274

Title: Electronic heat conductivity in a two-temperature state

Author(s): Medvedev, N (Medvedev, Nikita); Akhmetov, F (Akhmetov, Fedor); Milov, I (Milov, Igor)

Source: INTERNATIONAL JOURNAL OF HEAT AND MASS TRANSFER **Volume:** 228 **Article Number:** 125674 **DOI:** 10.1016/j.ijheatmasstransfer.2024.125674 **Early Access Date:** MAY 2024 **Published Date:** 2024 AUG 15

Abstract: Heat transport in solids is governed by two fundamental contributions, atomic and electronic. The electronic energy transport in transient excited states is a defining factor in the problem of ultrafast material irradiation. Here, we calculate the electronic heat conductivity at elevated electron temperatures up to 40,000 K. We apply the novel combined method of tight binding formalism to calculate the electron-phonon contribution to the electronic heat conductivity, and the linear response theory (in the single-pole Ritchie-Howie loss function approximation) for its electron-electron counterpart, implemented in the hybrid code XTANT-3. It allows us to evaluate the electronic heat conductivity in a wide range of materials - fcc metals: Al, Ca, Ni, Cu, Sr, Y, Zr, Rh, Pd, Ag, Ir, Pt, Au, and Pb; hcp metals: Mg, Sc, Ti, Co, Zn, Tc, Ru, Cd, Hf, Re, and Os; bcc metals: V, Cr, Fe, Nb, Mo, Ba, Ta, and W; other metals: Sn, Ga, In, Mn, Te, and Se; semimetal graphite; semiconductors - group IV: Si, Ge, and SiC; group III-V: AlAs, AlP, GaP, GaAs, and GaSb; oxides: ZnO, TiO2, and Cu2O; and others: PbI2, ZnS, and B4C.

Accession Number: WOS:001240935800001

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ISSN: 0017-9310

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Record 99 of 274

Title: Broadband thulium fiber amplifier for spectral region located beyond the L-band

Author(s): Aubrecht, J (Aubrecht, Jan); Pokorny, J (Pokorny, Jan); Svejkarová, B (Svejkarova, Bara); Kamrádek, M (Kamradek, Michal); Peterka, P (Peterka, Pavel)

Source: OPTICS EXPRESS **Volume:** 32 **Issue:** 10 **Pages:** 17932-17941 **DOI:** 10.1364/OE.522088 **Published Date:** 2024 MAY 6

Abstract: We present the development of a pair of silica -based thulium -doped fiber amplifiers working together in a broad spectral range from 1.65 mu m to 2.02 mu m. For the one optimized for shorter wavelengths, we designed and prepared optical fiber with a depressed cladding. We show the performance of the amplifiers achieving small -signal gain of at least 10 dB over 350 nm range from 1670 nm to 2020 nm, maximum gain of 40.7 dB with a noise figure as low as 6.45 dB and an optical signal-to-noise ratio of up to 50 dB. To the best of our knowledge, it is the first time that thulium fiber amplifiers of straightforward design without using redundant spectral filters operating efficiently in such a wide spectral region are demonstrated.

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PubMed ID: 38858961

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Peterka, Pavel	H-4298-2014	0000-0002-6341-7589
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ISSN: 1094-4087

Record 100 of 274

Title: Depressed-cladding thulium-doped fiber for below 1800 nm

Author(s): Pokorny, J (Pokorny, Jan); Aubrecht, J (Aubrecht, Jan); Kamrádek, M (Kamradek, Michal); Svejkarová, B (Svejkarova, Bara); Varák, P (Varak, Petr); Grábner, M (Grabner, Martin); Peterka, P (Peterka, Pavel)

Source: OPTICS EXPRESS **Volume:** 32 **Issue:** 10 **Pages:** 17966-17976 **DOI:** 10.1364/OE.523168 **Published Date:** 2024 MAY 6

Abstract: We present a thulium -doped silica fiber, featuring a depressed cladding, for applications at wavelengths below 1800 nm. The depressed cladding is used as a distributed filter suppressing amplified spontaneous emission at longer wavelengths, which helps promote emission at shorter wavelengths. We describe the fiber design process that was carried out by using a combination of numerical methods. The fiber was prepared in-house by a combination of the standard modified chemical vapor deposition method and nanoparticle doping. We demonstrate the effectiveness and tunability of ASE filtering, which

is influenced by fiber bend radius and its variation. (c) 2024 Optica Publishing Group under the terms of the Optica Open Access Publishing Agreement

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PubMed ID: 38858964

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Kamradek, Michal	KMA-7603-2024	
Svejkarova, Bara		0009-0006-3604-2319
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Varak, Petr		0000-0001-8026-0686
Peterka, Pavel	H-4298-2014	0000-0002-6341-7589

ISSN: 1094-4087

Record 101 of 274

Title: New markers for flowering-time selection in sweet cherry

Author(s): Holusová, K (Holusova, Katerina); Cmejlová, J (Cmejlova, Jana); Zdárská, I (Zdarska, Ivona); Suran, P (Suran, Pavol); Cmejla, R (Cmejla, Radek); Sedák, J (Sedlak, Jiri); Zeleny, L (Zeleny, Lubor); Bartos, J (Bartos, Jan)

Source: SCIENTIA HORTICULTURAE **Volume:** 332 **Article Number:** 113226 **DOI:** 10.1016/j.scienta.2024.113226 **Early Access Date:** APR 2024 **Published Date:** 2024 JUN 1

Abstract: Sweet cherry (Prunus avium L.) is a fruit tree in the Rosaceae family grown worldwide for its tasty fruit. However, its yield may be threatened in warmer growing regions by insufficient dormancy, which usually occurs in late-blooming genotypes. Conversely, in cold regions, the yield is threatened by late spring frosts, especially for early flowering cultivars. It is therefore necessary to breed cultivars adapted to local weather conditions and avoid potential crop losses. New markers associated with the beginning of flowering were sought to enable molecular marker-assisted selection of genotypes tailored for different climatic conditions. Previously whole-genome sequenced 298 sweet cherry genotypes with nine years of phenotypic evaluation provided the basis for a genome-wide association study that allowed the identification of 163 single nucleotide polymorphisms and indels associated with flowering time, located on all sweet cherry chromosomes. This study confirmed the previously predicted polygenic basis of the trait. Three markers suitable for selection of late-blooming genotypes and one for early-blooming genotypes were selected and validated using independent 128 sweet cherry hybrids from different crossings. Individual markers for late beginning of flowering were able to select genotypes flowering at least three days after the reference (i.e. the earliest flowering) cultivar 'Kisinevskaja'. Accumulation of preferred allele combinations for all three late-blooming markers has a synergistic effect, indicating delay of flowering 7.1 days after the reference cultivar on average. The marker for early beginning of flowering identified accessions flowering maximally five days after the earliest flowering reference cultivar 'Kisinevskaja'. All four markers were integrated into a single base extension assay to help breeders with prediction of beginning of flowering for their breeding materials and cultivars.

Accession Number: WOS:001236350300001

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Zelený, Lubor	AAF-7663-2021	
Suran, Pavol	AAP-5446-2020	
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Record 102 of 274

Title: Plant kleptomaniacs: geographical genetic patterns in the amphi-apomictic Rubus ser. Glandulosi (Rosaceae) reveal complex reticulate evolution of Eurasian brambles

Author(s): Sochor, M (Sochor, Michal); Sarhanova, P (Sarhanova, Petra); Duchoslav, M (Duchoslav, Martin); Konecna, M (Konecna, Michaela); Hrones, M (Hrones, Michal); Travnicek, B (Travnicek, Bohumil)

Source: ANNALS OF BOTANY **Volume:** 134 **Issue:** 1 **Pages:** 163-178 **DOI:** 10.1093/aob/mcae050 **Early Access Date:** APR 2024 **Published Date:** 2024 APR 12

Abstract: Background and Aims Rubus ser. Glandulosi provides a unique model of geographical parthenogenesis on a homoploid (2n = 4x) level. We aim to characterize evolutionary and phylogeographical patterns in this taxon and shed light on the geographical differentiation of apomicts and sexuals. Ultimately, we aim to evaluate the importance of phylogeography in the formation of geographical parthenogenesis.Methods Rubus ser. Glandulosi was sampled across its Eurasian range together with other co-occurring Rubus taxa (587 individuals in total). Double-digest restriction site-associated DNA sequencing (ddRADseq) and modelling of suitable climate were used for evolutionary inferences.Key Results Six ancestral species were identified that contributed to the contemporary gene pool of R. ser. Glandulosi. Sexuals were introgressed from Rubus dolichocarpus and Rubus moschus in West Asia and from Rubus ulmifolius agg., Rubus canescens and Rubus incanescens in Europe, whereas apomicts were characterized by alleles of Rubus subsect. Rubus. Gene flow between sexuals and apomicts was also detected, as was occasional hybridization with other taxa.Conclusions We hypothesize that sexuals survived the last glacial period in several large southern refugia, whereas apomicts were mostly restricted to southern France, whence they quickly recolonized Central and Western Europe. The secondary contact of sexuals and apomicts was probably the principal factor that established geographical parthenogenesis in R. ser. Glandulosi. Sexual populations are not impoverished in genetic diversity along their borderline with apomicts, and maladaptive population genetic processes probably did not shape the geographical patterns.

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PubMed ID: 38549558

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Record 103 of 274

Title: Five New Tamarixetin Glycosides from Astragalus thracicus Griseb. Including Some Substituted with the Rare 3-Hydroxy-3-methylglutaric Acid and Their Collagenase Inhibitory Effects In Vitro

Author(s): Vasilev, H (Vasilev, Hristo); Smejkal, K (Smejkal, Karel); Jusková, S (Juskova, Sabina); Vaclavik, J (Vaclavik, Jiri); Treml, J (Treml, Jakub)

Source: ACS OMEGA **Volume:** 9 **Issue:** 16 **Pages:** 18023-18031 **DOI:** 10.1021/acsomega.3c09677 **Early Access Date:** APR 2024 **Published Date:** 2024 APR 8

Abstract: Along with the known kaempferol-3-O-alpha-l-rhamnopyranosyl-(1 -> 2)-[6-O-(3-hydroxy-3-methylglutaryl)]-beta-d-galactopyranoside (1), five new flavonoids, containing the rarely isolated aglycon tamarixetin, were isolated from a methanolic extract of the endemic Balkan species Astragalus thracicus Griseb. Three of the new compounds are substituted with 3-hydroxy-3-methylglutaryl residue (HMG), untypical for the genus Astragalus. The compounds were identified as tamarixetin-3-O-alpha-l-rhamnopyranosyl-(1 -> 2)-[6-O-(3-hydroxy-3-methylglutaryl)]-beta-d-galactopyranoside (2), tamarixetin-3-O-(2,6-di-O-alpha-l-rhamnopyranosyl)-beta-d-galactopyranoside (3), tamarixetin 3-O-beta-d-apiofuranosyl-(1 -> 2)-beta-d-galactopyranoside (4), tamarixetin-3-O-beta-d-apiofuranosyl-(1 -> 2)-[6-O-(3-hydroxy-3-methylglutaryl)]-beta-d-galactopyranoside (5), and tamarixetin-3-O-beta-d-apiofuranosyl-(1 -> 2)-[alpha-l-rhamnopyranosyl-(1 -> 6)]-beta-d-galactopyranoside (6). Selected compounds from A. thracicus were tested to evaluate their anticollagenase activity. The greatest effect was observed for quercetin-3-O-beta-d-apiofuranosyl-(1 -> 2)-beta-d-galactopyranoside, possibly due to the presence of an ortho-dihydroxy arrangement of flavonoid ring B. The effect on collagenase and elastase was further evaluated also by in silico study, and the test compounds showed some level of in silico interaction.

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PubMed ID: 38680358

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ISSN: 2470-1343

Record 104 of 274

Title: Mast Cells in the Microenvironment of Hepatocellular Carcinoma Confer Favorable Prognosis: A Retrospective Study using QuPath Image Analysis Software

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Source: JOVE-JOURNAL OF VISUALIZED EXPERIMENTS **Issue:** 206 **Article Number:** e66743 **DOI:** 10.3791/66743 **Published Date:** 2024 APR

Abstract: The insights provided by in -situ detection of immune cells within hepatocellular carcinoma (HCC) might present information on patient outcomes. Studies investigating the expression and localization of immune cells within tumor tissues are associated with several challenges, including a lack of precise annotation for tumor regions and random selection of microscopic fields of view. QuPath is an open -source, user-friendly software that could meet the growing need for digital pathology in wholeslide image (WSI) analysis. The infiltration of HCC and adjacent tissues by CD1a+ immature dendritic cells (iDCs), CD117+ mast cells, and NKp46+ natural killer cells (NKs) cells was assessed immunohistochemically in representative specimens of 67 patients with HCC who underwent curative resection. The area fraction (AF) of positively stained cells was assessed automatically in WSIs using QuPath in the tumor center (TC), inner margin (IM), outer margin (OM), and peritumor (PT) area. The prognostic significance of immune cells was evaluated for time to recurrence (TTR), disease -free survival (DFS), and overall survival (OS). The AF of mast cells was significantly greater than the AF of NKs, and the AF of iDCs was significantly lower compared to NKs in each region of interest. High AFs of mast cells in the IM and PT areas were associated with longer DFS. In addition, high AF of mast cells

in IM was associated with longer OS. Computer -assisted analysis using this software is a suitable tool for obtaining prognostic information for tumor -infiltrating immune cells (iDCs, mast cells, and NKs) in different regions of HCC after resection. Mast cells displayed the greatest AF in all regions of interest (ROIs). Mast cells in the peritumor region and IM showed a positive prognostic significance.

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PubMed ID: 38682951

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ISSN: 1940-087X

Record 105 of 274

Title: Formation of Ar₂⁺ ions in cold argon plasmas through the ternary recombination mechanism

Author(s): Nongni, FT (Nongni, F. T.); Kalus, R (Kalus, R.); Benhenni, M (Benhenni, M.); Gadéa, FX (Gadea, F. X.); Yousfi, M (Yousfi, M.)

Source: PLASMA SOURCES SCIENCE & TECHNOLOGY **Volume:** 33 **Issue:** 4 **Article Number:** 045011 **DOI:** 10.1088/1361-6595/ad377a **Published Date:** 2024 APR 1

Abstract: A general scheme for calculating ternary recombination rate constants of atomic species based on a hybrid quantum-classical nonadiabatic dynamics approach is presented and applied to the specific case of the ternary recombination of atomic ions of argon in cold argon plasmas. Rate constants are reported for both fine-structure states of the Ar + ion,P- 2(3/2) and(2)P(1/2), T = 300 K, and for selected values of the reduced electric field. A thorough comparison with the literature data available for T = 300 K and a couple of close temperatures is performed with a favorable agreement achieved. It is shown that the excited Ar + (P-2 (1/2)) ions may contribute to the formation of dimer ions, Ar-2(+) , as efficiently as the ground-state ions, Ar + (P-2(3/2)) , due to fast internal conversion of the electronic energy, which takes place in ternary collision complexes, Ar (+) / Ar / Ar .

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Record 106 of 274

Title: Defect-induced properties of MoSi₂/Nb(Ta)Si₂ disilicide nanocomposites

Author(s): Vsianská, M (Vsianska, Monika); Pavlu, J (Pavlu, Jana); Sob, M (Sob, Mojmir)

Source: MATERIALS TODAY COMMUNICATIONS **Volume:** 39 **Article Number:** 108584 **DOI:** 10.1016/j.mtcomm.2024.108584 **Early Access Date:** MAR 2024 **Published Date:** 2024 JUN

Abstract: Research on disilicide nanocomposites, as modern materials with promising technological applications, is very desirable these days. Our ab initio analysis concentrates on the C11(b) (tetragonal) MoSi2/C40 (hexagonal) NbSi2 or TaSi2 nanocomposites containing 12 types of interfaces formed by (110) planes in the C11(b) and (0001) planes in the C40 disilicide. The most stable nanocomposites are MoSi2(AC)/Nb(Ta)Si-2(BAC), MoSi2(AB)/Nb(Ta)Si-2(CAB) and MoSi2(AB)/Nb(Ta)Si-2(ABC). The interfaces reveal positive formation energies, e.g. gamma(BA)(IF) = 0.63670 J.m(-2) and gamma(CA)(IF) = 0.63727 J.m(-2) in the Nb system and gamma(BA)(IF) = 0.57837 J.m(-2) and gamma(CA)(IF) = 0.57802 J.m(-2) in the Ta system. In the most stable C(11)b-MoSi2(AC)/C40-Nb(Ta)Si-2(BAC) nanocomposite, the effect of the impurities (Al, Si), vacancies or their aggregates on the stability and structure is investigated. It turns out that (i) vacancies preferentially form at the Si positions in the third (first) layer of MoSi2 in the Nb (Ta) systems, utilising an energy of 2.259 eV.Va(-1) (1.971 eV. Va(-1));

(ii) Al impurities prefer Si positions, and it is easier to introduce them into the Ta system than into the Nb one; however, this does not apply if Al is in the Mo position; (iii) Si impurities prefer Ta positions to Nb ones, and the bulk to interfacial ones; (iv) the Si-Si divacancy is the least destabilising among divacancies; and (v) Al impurities in both systems prevent the formation of Si vacancies, and the Si impurities simplify the formation of vacancies in the Nb system. As there is very little experimental information on the structure and properties of these interfaces, most of the present results are theoretical predictions which may motivate future experimental work.

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eISSN: 2352-4928

Record 107 of 274

Title: Charge-induced ultralow friction between graphite and atomically flat surfaces

Author(s): Liao, MZ (Liao, Mengzhou); Cammarata, A (Cammarata, Antonio); Polcar, T (Polcar, Tomas)

Source: CARBON **Volume:** 223 **Article Number:** 119036 **DOI:** 10.1016/j.carbon.2024.119036 **Early Access Date:** MAR 2024 **Published Date:** 2024 APR 10

Abstract: Reaching near-zero friction is one of the jewels on the crown of tribology, and structural superlubricity is a crucial mechanism to achieve it. Previous works focus mainly on the structural superlubricity at incommensurate crystalline interfaces. However, realizing such interfaces on a large scale without defects and contaminations is a formidable challenge. Here, we report a charge-induced robust macroscale superlubricity between graphite and atomically flat surfaces in the ambient condition. We transferred graphite flakes on Si3N4 balls and used them to measure the friction properties on pristine and charged atomically flat surfaces such as 300 nm SiO2/Si and sapphire. We found that the surface charge can dramatically reduce the coefficient of friction between graphite and substrates by two orders of magnitude to 10(-4), and the sliding is wearless even under harsh contact conditions (similar to 1.1 GPa center pressure and >100 m). We demonstrate that the surface charge is critical in achieving superlubricity possibly because it can reduce adhesion between graphite and substrate surfaces and make the substrate surfaces resistant to contaminations. Our method offers a ready-to-use solution to superlubricity alternative to achieve incommensurate crystalline interfaces. Thus, it can reduce the difficulty of realizing macroscale superlubricity for applications.

Accession Number: WOS:001219295000001

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Record 108 of 274

Title: The preparation route and final form of V-MXenes override the effect of the O/F ratio on their magnetic properties

Author(s): Eliášová, P (Eliasova, Pavla); Smíd, B (Smid, Bretislav); Vejpravová, J (Vejpravova, Jana); Li, S (Li, Shuo); Brivio, F (Brivio, Federico); Mazur, M (Mazur, Michal); Rainer, DN (Rainer, Daniel N.); Mohideen, MIH (Mohideen, M. Infas H.); Morris, RE (Morris, Russell E.); Nachtigall, P (Nachtigall, Petr)

Source: JOURNAL OF MATERIALS CHEMISTRY C **Volume:** 12 **Issue:** 15 **Pages:** 5431-5441 **DOI:** 10.1039/d4tc00132j **Early Access Date:** MAR 2024 **Published Date:** 2024 APR 18

Abstract: Transition metal carbides and nitrides (MXenes) show a high potential for electrochemical energy storage in batteries and supercapacitors and for electrocatalysis. Their excellent electronic and magnetic characteristics have been highlighted in several theoretical studies. However, experimental research on MXenes is yet to confirm their predicted properties as candidates for controllable magnetic 2D materials. Here, we report our theoretical and experimental study of V2CTx MXenes (T = O, OH, F), providing key insights into their magnetism. Based on our density functional theory (DFT) analysis, we predicted ferromagnetic (FM) and antiferromagnetic (AFM) states of V2CTx, which are determined by the O/F ratio of surface functional groups. Accordingly, we prepared V2CTx MXenes in the form of multilayered powders and thin films with different O/F ratios. No experimental evidence of FM or AFM properties was found in any material. Nevertheless, powders and films with almost identical chemical compositions (in terms of O/F ratio) displayed different magnetic properties, whereas films with disparate chemical compositions revealed a similar magnetic character. Therefore, the preparation route and form of the final V2CTx material override the effect of the O/F ratio, which is often overestimated in theoretical studies. Moreover, these findings underscore the importance of preparing MXene materials to experimentally confirm their theoretically predicted properties.
A theoretical and experimental study of V2CTx provides key insights into its magnetism. Chemical analysis and magnetic measurements highlight the importance of the preparation pathway rather than the actual chemical composition and form of V2CTx.

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Record 109 of 274

Title: Zinc priming enhances Capsicum annuum immunity against infection by Botrytis cinerea- From the whole plant to the molecular level

Author(s): Kuvelja, A (Kuvelja, Andela); Morina, F (Morina, Filis); Mijovilovich, A (Mijovilovich, Ana); Bokhari, SNH (Bokhari, Syed Nadeem Hussain); Konik, P (Konik, Peter); Koloniuk, I (Koloniuk, Igor); Küpper, H (Kupper, Hendrik)

Source: PLANT SCIENCE **Volume:** 343 **Article Number:** 112060 **DOI:** 10.1016/j.plantsci.2024.112060 **Early Access Date:** MAR 2024 **Published Date:** 2024 JUN

Abstract: Micronutrient manipulation can enhance crop resilience against pathogens, but the mechanisms are mostly unknown. We tested whether priming Capsicum annuum plants with zinc (5 mu M Zn) or manganese (3 mu M Mn) for six weeks increases their immunity against the generalist necrotroph Botrytis cinerea compared to deficient (0.1 mu M Zn, 0.02 mu M Mn) and control conditions (1 mu M Zn, 0.6 mu M Mn). Zinc priming reduced the pathogen biomass and lesion area and preserved

CO 2 assimilation and stomatal conductance. Zinc mobilization at the infection site, visualized by micro-X-ray fluorescence, was accompanied by increased Zn protein binding obtained by size exclusion HPLC-ICP/MS. A common metabolic response to fungal infection in Zn- and Mn-primed plants was an accumulation of corchorifatty acid F, a signaling compound, and the antifungal compound acetophenone. In vitro tests showed that the binding of Zn 2 + increased, while Mn 2 + binding decreased acetophenone toxicity against B. cinerea at concentrations far below the toxicity thresholds of both metals in unbound (aquo complex) form. The metal-specific response to fungal infection included the accumulation of phenolics and amino acids (Mn), and the ligand isocitrate (Zn). The results highlight the importance of Zn for pepper immunity through direct involvement in immunity-related proteins and low molecular weight Zn-complexes, while Mn priming was inefficient.

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PubMed ID: 38460554

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Record 110 of 274

Title: Small-scale regional engineering geological study of the Czech Republic evaluating the relationship between slope gradients and engineering geological zones

Author(s): Marschalko, M (Marschalko, Marian); Zieba, Z (Zieba, Zofia); Ruzicková, K (Ruzickova, Katerina); Ruzicka, J (Ruzicka, Jan); Kubac, J (Kubac, Jan); Dabrowska, J (Dabrowska, Jolanta); Sysala, D (Sysala, David); Krcmár, D (Krcmar, David)

Source: SCIENTIFIC REPORTS **Volume:** 14 **Issue:** 1 **Article Number:** 5507 **DOI:** 10.1038/s41598-024-55972-z **Published Date:** 2024 MAR 6

Abstract: The aim of the small-scale regional engineering geological study of the Czech Republic was to evaluate the relationship between slope gradient and engineering geological zones. The research motivation was to determine the average slope gradient, 25%, 50% (median) and 75% quantiles related to the different engineering geological zones. This scientific information is critical from the perspectives of engineering geology, geotechnical engineering, and foundation engineering because an increasing slope gradient evokes the need to create a cut respectively foundation excavation or another excavation in the geological structure, which increases the probability of occurrence of the problem in terms of differential settlement and bearing capacity of the structures. The research was carried out in the territory of the Czech Republic in 8 Quaternary zones with soil foundation ground and 10 pre-Quaternary zones with rocks and semi-rocks and their eluvia. A significant difference in the statistical characteristics of slope gradients was found in the group of Quaternary engineering geological zones (evaluated group I) compared to the group of pre-Quaternary zones (evaluated group II). The value range of the average slope gradient was 1.65 degrees (16.9%) to 5.89 degrees (60.3%) for the Quaternary engineering geological zones (soil foundation ground), representing 43.4% difference. Whereas for the over-quaternary engineering geological zones (rocks, semi-rocks and their eluvia), the difference was much higher, 3.59 degrees (36.8%) to 9.76 degrees (100%-value determined as a referential because it was the maximum), which is also reflected in a more significant percentage difference of 63.2%.

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PubMed ID: 38448572

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ISSN: 2045-2322

Record 111 of 274

Title: Parametric analysis of electron beam quality in laser wakefield acceleration based on the truncated ionization injection mechanism

Author(s): Maity, S (Maity, Srimanta); Mondal, A (Mondal, Alamgir); Vishnyakov, E (Vishnyakov, Eugene); Molodozhentsev, A (Molodozhentsev, Alexander)

Source: PLASMA PHYSICS AND CONTROLLED FUSION **Volume:** 66 **Issue:** 3 **Article Number:** 035012 **DOI:** 10.1088/1361-6587/ad238e **Published Date:** 2024 MAR 1

Abstract: Laser wakefield acceleration (LWFA) in a gas cell target separating injection and acceleration section has been investigated to produce high-quality electron beams. A detailed study has been performed on controlling the quality of accelerated electron beams using a combination of truncated ionization and density downramp injection mechanisms. For this purpose, extensive two-dimensional particle-in-cell simulations have been carried out considering a gas cell target consisting of a hydrogen and nitrogen mixture in the first part and pure hydrogen in the second part. Such a configuration can be realized experimentally using a specially designed capillary setup. Using the parameters already available in the existing experimental setups, we show the generation of an electron beam with a peak energy of 500-600 MeV, relative energy spread less than 5% , normalized beam emittance around 1.5 mm-mrad, and beam charge of 2-5 pC/mu m. Our study reveals that the quality of the accelerated electron beam can be independently controlled and manipulated through the beam loading effect by tuning the parameters, e.g. laser focusing position, nitrogen concentration, and gas target profile. These simulation results will be useful for future experimental campaigns on LWFA, particularly at ELI Beamlines.

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Record 112 of 274

Title: In silico prediction of the metabolism of Blastocrithidia nonstop, a trypanosomatid with non-canonical genetic code

Author(s): Opperdoes, FR (Opperdoes, Fred R.); Záhonová, K (Zahonova, Kristina); Skodová-Sveráková, I (Skodova-Sverakova, Ingrid); Buckova, B (Buckova, Barbora); Chmelová, L (Chmelova, Lubomira); Lukes, J (Lukes, Julius); Yurchenko, V (Yurchenko, Vyacheslav)

Source: BMC GENOMICS **Volume:** 25 **Issue:** 1 **Article Number:** 184 **DOI:** 10.1186/s12864-024-10094-8 **Published Date:** 2024 FEB 16

Abstract: Background Almost all extant organisms use the same, so-called canonical, genetic code with departures from it being very rare. Even more exceptional are the instances when a eukaryote with non-canonical code can be easily cultivated and has its whole genome and transcriptome sequenced. This is the case of Blastocrithidia nonstop, a trypanosomatid flagellate that reassigned all three stop codons to encode amino acids. Results We in silico predicted the metabolism of B. nonstop and compared it with that of the well-studied human parasites Trypanosoma brucei and Leishmania major. The mapped mitochondrial, glycosomal and cytosolic metabolism contains all typical features of these diverse and important parasites. We also provided experimental validation for some of the predicted observations, concerning, specifically presence of glycosomes, cellular respiration, and assembly of the respiratory complexes. Conclusions In an unusual comparison of metabolism between a parasitic protist with a massively altered genetic code and its close relatives that rely on a canonical code we showed that the dramatic differences on the level of nucleic acids do not seem to be reflected in the metabolisms. Moreover, although the genome of B. nonstop is extremely AT-rich, we could not find any alterations of its pyrimidine synthesis pathway when compared to other trypanosomatids. Hence, we conclude that the dramatic alteration of the genetic code of B. nonstop has no significant repercussions on the metabolism of this flagellate.

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PubMed ID: 38365628

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Sverakova, Ingrid		0000-0002-4004-3377

ISSN: 1471-2164

Record 113 of 274

Title: Oxygen exchange mechanisms in zeolite chabazite under steaming conditions

Author(s): Benes, T (Benes, Tereza); Liu, MX (Liu, Mingxiu); Nachtigall, P (Nachtigall, Petr); Heard, CJ (Heard, Christopher J.)

Source: MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 368 **Article Number:** 113007 **DOI:** 10.1016/j.micromeso.2024.113007 **Early Access Date:** FEB 2024 **Published Date:** 2024 MAR 15

Abstract: Under hydrothermal conditions, zeolite frameworks can readily incorporate oxygen from water, via reactive oxygen exchange. This indicates that zeolite frameworks are highly labile and reactive to water, even when stable against full hydrolytic dissolution. However, the routes by which oxygen is exchanged between water and framework have not been established. In this work, we identify the preferable oxygen exchange mechanisms in the zeolite chabazite (CHA) and compare them to hydrolysis and other framework healing mechanisms under the low water concentrations relevant for steaming conditions. We find that oxygen exchange occurs at defect sites that are created by the first hydrolysis step, both in Al-O and Si-O bonds and is competitive with subsequent hydrolysis and non-exchange framework healing processes. Furthermore, we determine the effect of increased water concentration, finding that for both Al-O and Si-O bonds, the second water can either moderately enhance or hinder both hydrolysis and O-exchange, depending on the geometry of the site. This implies that local water

concentration is an important factor with varied effects on zeolite stability as a function of water loading. This work provides feasible routes of oxygen exchange in CHA, which together with hydrolytic pathways, govern the stability and mesoporosity of these important porous materials.

Accession Number: WOS:001175825800001

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Record 114 of 274

Title: Comprehensive experimental and numerical validation of Lattice Boltzmann fluid flow and particle simulations in a child respiratory tract

Author(s): Prinz, F (Prinz, Frantisek); Pokorny, J (Pokorny, Jan); Elcner, J (Elcner, Jakub); Lízal, F (Lizal, Frantisek); Misík, O (Misik, Ondrej); Maly, M (Maly, Milan); Belka, M (Belka, Miloslav); Hafen, N (Hafen, Nicolas); Kummerländer, A (Kummerlaender, Adrian); Krause, MJ (Krause, Mathias J.); Jedelsky, J (Jedelsky, Jan); Jícha, M (Jicha, Miroslav)

Source: COMPUTERS IN BIOLOGY AND MEDICINE **Volume:** 170 **Article Number:** 107994 **DOI:** 10.1016/j.compbiomed.2024.107994 **Early Access Date:** FEB 2024 **Published Date:** 2024 MAR

Abstract: The numerical simulation of inhaled aerosols in medical research starts to play a crucial role in understanding local deposition within the respiratory tract, a feat often unattainable experimentally. Research on children is particularly challenging due to the limited availability of in vivo data and the inherent morphological intricacies. CFD solvers based on Finite Volume Methods (FVM) have been widely employed to solve the flow field in such studies. Recently, Lattice Boltzmann Methods (LBM), a mesoscopic approach, have gained prominence, especially for their scalability on High -Performance Computers. This study endeavours to compare the effectiveness of LBM and FVM in simulating particulate flows within a child's respiratory tract, supporting research related to particle deposition and medication delivery using LBM. Considering a 5 -year -old child's airway model at a steady inspiratory flow, the results are compared with in vitro experiments. Notably, both LBM and FVM exhibit favourable agreement with experimental data for the mean velocity field and the turbulence intensity. For particle deposition, both numerical methods yield comparable results, aligning well with in vitro experiments across a particle size range of 0.1-20 mu m. Discrepancies are identified in the upper airways and trachea, indicating a lower deposition fraction than in the experiment. Nonetheless, both LBM and FVM offer invaluable insights into particle behaviour for different sizes, which are not easily achievable experimentally. In terms of practical implications, the findings of this study hold significance for respiratory medicine and drug delivery systems - potential health impacts, targeted drug delivery strategies or optimisation of respiratory therapies.

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PubMed ID: 38308867

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Record 115 of 274

Title: Formation of ethane by activation of methane on B, N co-doped graphene surface decorated by Ir13 cluster: A first principle study

Author(s): Damte, JY (Damte, Jemal Yimer); Hailu, YM (Hailu, Yohannes Mulugeta); Cammarata, A (Cammarata, Antonio)

Source: APPLIED SURFACE SCIENCE **Volume:** 654 **Article Number:** 159524 **DOI:** 10.1016/j.apsusc.2024.159524 **Early Access Date:** FEB 2024 **Published Date:** 2024 MAY 1

Abstract: The most critical processes in designing a potential catalyst for the production of ethane are activating methane and suppressing further dehydrogenation. In the present study, using first- principle calculations, we predict that the BNG-Ir13 cluster can efficiently activate methane and promote the C-C coupling reactions. Ir in the BNGIr13 cluster's top site is found to be the most stable adsorption site of methane with stable adsorption energy of -0.45 eV. Methane is activated with a low activation energy barrier of 0.16 eV, and the reaction energy is -0.54 eV. It is the most facile step and is thermodynamically favorable, likely to occur at low-temperature conditions. The fourth dehydrogenation step is the rate-determining step, which shows the highest activation energy barrier (1.24 eV) in the methane dehydrogenation process on the BNG- Ir13 cluster. Based on the DFT calculations, selective dehydrogenation of methane and self- coupling reactions of methyl groups formed ethane with a low kinetic barrier assisted by the BNG-Ir13 cluster. Furthermore, hydrogen molecules are likely to form, implying that the BNG-Ir13 cluster is a potential and bi-functional catalyst in selective conversion of methane to ethane and in the production of hydrogen molecules at optimum conditions.

Accession Number: WOS:001176590900001

Author Identifiers:

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ISSN: 0169-4332

eISSN: 1873-5584

Record 116 of 274

Title: Examining the co-occurrences of human threats within terrestrial protected areas

Author(s): Martini, F (Martini, Francesco); Kounnamas, C (Kounnamas, Constantinos); Goodale, E (Goodale, Eben); Mammides, C (Mammides, Christos)

Source: AMBIO **DOI:** 10.1007/s13280-023-01966-6 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN 25

Abstract: Human threats to biodiversity are prevalent within protected areas (PAs), undermining their effectiveness in halting biodiversity loss. Certain threats tend to co-occur, resulting in amplified cumulative impact through synergistic effects. However, it remains unclear which threats are related the most. We analyzed a dataset of 71 human threats in 18 013 terrestrial PAs of the European Union's Natura 2000 network, using a Joint Species Distribution Modelling approach, to assess the threats' co-occurrence patterns and potential drivers. Overall, threats were more frequently correlated positively than negatively. Threats related to agriculture and urbanization were correlated strongly with most other threats. Approximately 70% of the variance in our model was explained by country-specific factors, indicating the importance of local drivers. Minimizing the negative impact of key threats can likely reduce the impact of related threats. However, more research is needed to understand better the relationships among threats and, importantly, their combined impact on biodiversity.

Accession Number: WOS:001148265400002

PubMed ID: 38273093

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Mammides, Christos	H-4194-2019	0000-0003-1747-175X

ISSN: 0044-7447

eISSN: 1654-7209

Record 117 of 274

Title: Magnetization dynamics induced by ultrashort terahertz radiation: Toward designing spin-based terahertz sensors

Author(s): Korniienko, I (Korniienko, I.); Nieves, P (Nieves, P.); Chubykalo-Fesenko, O (Chubykalo-Fesenko, O.); Legut, D (Legut, D.)

Source: PHYSICAL REVIEW APPLIED **Volume:** 21 **Issue:** 1 **Article Number:** 014025 **DOI:** 10.1103/PhysRevApplied.21.014025 **Published Date:** 2024 JAN 16

Abstract: A convenient analytical description of an ultrashort terahertz pulse and an analysis of the influence of this pulse on the Zeeman torque dynamics are extremely important tasks due to the potential applications of terahertz radiation. The theoretical expressions proposed in this paper clarify the physics of magnetic dynamics under the action of the magnetic field of a terahertz pulse and show the role of individual parameters of the material and the pulse field in this process. On the basis of the formulas obtained and the available experimental data for fcc-Co film, we analyze the possibilities of recovering information about the magnetic field of the pulse from the observation of magnetization dynamics, as well as the effect of fluence, Gilbert damping, and magnetic anisotropy on the magnetization dynamics induced by ultrashort terahertz radiation. The theoretical framework presented could potentially be used in the design and optimization of a new generation of terahertz detectors based on the magnetic component of the electromagnetic field.

Accession Number: WOS:001158820500002

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Nieves, Pablo	GZG-1849-2022	
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Korniienko, Ievgeniia	AAK-4126-2020	
Korniienko, Ievgeniia		0000-0003-3051-120X

Chubykalo-Fesenko, Oksana	V-5015-2017	0000-0002-4081-1831
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Nieves, Pablo		0000-0002-6633-9643

ISSN: 2331-7019

Record 118 of 274

Title: Microbial, proteomic, and metabolomic profiling of the estrous cycle in wild house mice

Author(s): Matejková, T (Matejkova, Tereza); Dodoková, A (Dodokova, Alica); Kreisinger, J (Kreisinger, Jakub); Stopka, P (Stopka, Pavel); Stopková, R (Stopkova, Romana)

Source: MICROBIOLOGY SPECTRUM **Volume:** 12 **Issue:** 2 **DOI:** 10.1128/spectrum.02037-23 **Early Access Date:** JAN 2024 **Published Date:** 2024 FEB 6

Abstract: Symbiotic microbial communities affect the host immune system and produce molecules contributing to the odor of an individual. In many mammalian species, saliva and vaginal fluids are important sources of chemical signals that originate from bacterial metabolism and may act as honest signals of health and reproductive status. In this study, we aimed to define oral and vaginal microbiomes and their dynamics throughout the estrous cycle in wild house mice. In addition, we analyzed a subset of vaginal proteomes and metabolomes to detect potential interactions with microbiomes. 16S rRNA sequencing revealed that both saliva and vagina are dominated by Firmicutes and Proteobacteria but differ at the genus level. The oral microbiome is more stable during the estrous cycle and most abundant bacteria belong to the genera Gemella and Streptococcus, while the vaginal microbiome shows higher bacterial diversity and dynamics during the reproductive cycle and is characterized by the dominance of Muribacter and Rodentibacter. These two genera cover around 50% of the bacterial community during estrus. Proteomic profiling of vaginal fluids revealed specific protein patterns associated with different estrous phases. Highly expressed proteins in estrus involve the keratinization process thus providing estrus markers (e.g., Hrnr) while some proteins are downregulated such as immune-related proteins that limit bacterial growth (Camp, Clu, Elane, Lyz2, and Ngp). The vaginal metabolome contains volatile compounds potentially involved in chemical communication, for example, ketones, aldehydes, and esters of carboxylic acids. Data integration of all three OMICs data sets revealed high correlations, thus providing evidence that microbiomes, host proteomes, and metabolomes may interact.IMPORTANCE Our data revealed dynamic changes in vaginal, but not salivary, microbiome composition during the reproductive cycle of wild mice. With multiple OMICs platforms, we provide evidence that changes in microbiota in the vaginal environment are accompanied by changes in the proteomic and metabolomics profiles of the host. This study describes the natural microbiota of wild mice and may contribute to a better understanding of microbiome-host immune system interactions during the hormonal and cellular changes in the female reproductive tract. Moreover, analysis of volatiles in the vaginal fluid shows particular substances that can be involved in chemical communication and reproductive behavior.

Accession Number: WOS:001135896200001

PubMed ID: 38171017

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kreisinger, Jakub	H-4020-2011	
Kreisinger, Jakub		0000-0001-9375-9814

ISSN: 2165-0497

Record 119 of 274

Title: Long-term (1951-2023) surface changes of the Belvedere Glacier observed through aerial and UAV orthophotos

Author(s): Azzoni, RS (Azzoni, Roberto Sergio); Bollati, IM (Bollati, Irene Maria); Pelfini, M (Pelfini, Manuela); Valzasina, S (Valzasina, Stefano); Brodsky, L (Brodsky, Lukas)

Source: AUC GEOGRAPHICA **Volume:** 59 **Issue:** 2 **Pages:** 203-213 **DOI:** 10.14712/23361980.2024.23 **Published Date:** 2024

Abstract: Glacier retreat is a key indicator of climate change, with significant implications for geomorphological hazards and ecosystem stability. This article focuses on the surface evolution of the Belvedere Glacier from 1951 to 2023. Using high-resolution orthophotos and manual mapping, we tracked changes in the glacier's area and shape over time. The results show three significant phases of change: the separation of the Nordend Glacier from the Belvedere Glacier (1951-1991), the partial separation of the central accumulation basin from the debris-covered tongue (2006-2015), and the separation of the Locce Nord Glacier (2018-2021). These changes, combined with a surge event from 1999 to 2002, have significantly altered the glacier's dynamics and accelerated its retreat. Manual mapping was accurate in areas with scarce debris cover but faced challenges in debris-covered areas due to limited image resolution, snow cover, and debris characteristics. Despite these difficulties, we observed that the glacier remained stable until the late 1990s, when it began a rapid retreat. This recent retreat is consistent with rates observed in the early 20th century. The study highlights the importance of surface mapping to quantify the areal loss and to understand broader changes in glacier structure and mass flow that drive its retreat. Our results provide key data for future studies and highlight the need for continued monitoring of Alpine glaciers in the context of accelerating climate change.

Accession Number: WOS:001389003400002

ISSN: 0300-5402

eISSN: 2336-1980

Record 120 of 274

Title: Security Implications of Deepfakes in Face Authentication

Author(s): Salko, M (Salko, Milan); Firc, A (Firc, Anton); Malinka, K (Malinka, Kamil)

Book Group Author(s): ASSOC COMPUTING MACHINERY

Source: 39TH ANNUAL ACM SYMPOSIUM ON APPLIED COMPUTING, SAC 2024 **Pages:** 1376-1384 **DOI:** 10.1145/3605098.3635953 **Published Date:** 2024

Abstract: Deepfakes are media generated by deep learning and are nearly indistinguishable from real content to humans. Deepfakes have seen a significant surge in popularity in recent years. There have been numerous papers discussing their effectiveness in deceiving people. What's equally, if not more concerning, is the potential vulnerability of facial and voice recognition systems to deepfakes. The misuse of deepfakes to spoof automated facial recognition systems can threaten various aspects of our lives, including financial security and access to secure locations. This issue remains largely unexplored. Thus, this paper investigates the technical feasibility of a spoofing attack on facial recognition. Firstly, we perform a threat analysis to understand what facial recognition use cases allow the execution of deepfake spoofing attacks. Based on this analysis, we define the attacker model for these attacks on facial recognition systems. Then, we demonstrate the ability of deepfakes to spoof two commercial facial recognition systems. Finally, we discuss possible means to prevent such spoofing attacks.

Accession Number: WOS:001236958200199

Conference Title: 39th Annual ACM Symposium on Applied Computing (SAC)

Conference Date: APR 08-12, 2024

Conference Location: Univ Salamanca, Avila, SPAIN

Conference Sponsors: Assoc Comp Machinery, ACM Special Interest Grp Appl Comp

Conference Host: Univ Salamanca

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ISBN: 979-8-4007-0243-3

Record 121 of 274

Title: Learning Not to Regret

Author(s): Sychrovsky, D (Sychrovsky, David); Sustr, M (Sustr, Michal); Davoodi, E (Davoodi, Elnaz); Bowling, M (Bowling, Michael); Lanctot, M (Lanctot, Marc); Schmid, M (Schmid, Martin)

Edited by: Wooldridge M; Dyl J; Natarajan S

Source: THIRTY-EIGHTH AAAI CONFERENCE ON ARTIFICIAL INTELLIGENCE, VOL 38 NO 14 **Book Series:** AAAI Conference on Artificial Intelligence **Pages:** 15202-15210 **Published Date:** 2024

Abstract: The literature on game-theoretic equilibrium finding predominantly focuses on single games or their repeated play. Nevertheless, numerous real-world scenarios feature playing a game sampled from a distribution of similar, but not identical games, such as playing poker with different public cards or trading correlated assets on the stock market. As these similar games feature similar equilibra, we investigate a way to accelerate equilibrium finding on such a distribution. We present a novel "learning not to regret" framework, enabling us to meta-learn a regret minimizer tailored to a specific distribution. Our key contribution, Neural Predictive Regret Matching, is uniquely meta-learned to converge rapidly for the chosen distribution of games, while having regret minimization guarantees on any game. We validated our algorithms' faster convergence on a distribution of river poker games. Our experiments show that the meta-learned algorithms outpace their non-meta-learned counterparts, achieving more than tenfold improvements.

Accession Number: WOS:001239983500003

Conference Title: 38th AAAI Conference on Artificial Intelligence (AAAI) / 36th Conference on Innovative Applications of Artificial Intelligence / 14th Symposium on Educational Advances in Artificial Intelligence

Conference Date: FEB 20-27, 2024

Conference Location: Vancouver, CANADA

Conference Sponsors: Assoc Advancement Artificial Intelligence

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Davoodi, Elnaz	HHN-3827-2022	

ISSN: 2159-5399

eISSN: 2374-3468

Record 122 of 274

Title: Global Aromatic Ring Currents in Neutral Porphyrin Nanobelts

Author(s): Vitek, M (Vitek, Marco); Deng, JR (Deng, Jie-Ren); Anderson, HL (Anderson, Harry L.); Roncevic, I (Roncevic, Igor)

Source: ACS NANO **DOI:** 10.1021/acsnano.4c14100 **Early Access Date:** DEC 2024 **Published Date:** 2024 DEC 31

Abstract: The ability of a ring-shaped molecule to sustain a global aromatic or antiaromatic ring current when placed in a magnetic field indicates that its electronic wave function is coherently delocalized around its whole circumference. Large molecules that display this behavior are attractive components for molecular electronic devices, but this phenomenon is rare in neutral molecules with circuits of more than 40 pi-electrons. Here, we use theoretical methods to investigate how the global ring currents evolve with increasing ring size in cyclic molecular nanobelts built from edge-fused porphyrins. Our results indicate that a global ring current persists in neutral nanobelts with Huckel circuits of 220 pi-electrons (22

porphyrin units, circumference 18.6 nm). Our predictions are validated by using coupled clusters to construct a density functional approximation (denoted as OX-B3LYP) that accurately describes these nanobelts and by checking compliance with Koopmans' theorem.

Accession Number: WOS:001387041700001

PubMed ID: 39810377

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Anderson, Harry	E-7843-2011	
Rončević, Igor	ABA-5332-2020	

ISSN: 1936-0851

eISSN: 1936-086X

Record 123 of 274

Title: Novel derivative operational matrix in Caputo sense with applications

Author(s): Zaidi, D (Zaidi, Danish); Talib, I (Talib, Imran); Riaz, MB (Riaz, Muhammad Bilal); Agarwal, P (Agarwal, Parveen)

Source: JOURNAL OF TAIBAH UNIVERSITY FOR SCIENCE **Volume:** 18 **Issue:** 1 **Article Number:** 2333061 **DOI:** 10.1080/16583655.2024.2333061 **Published Date:** 2024 DEC 31

Abstract: The main objective of this study is to present a computationally efficient numerical method for solving fractional-order differential equations with initial conditions. The proposed method is based on the newly developed generalized derivative operational matrix and generalized integral operational matrix derived from Laguerre polynomials, which belong to the class of orthogonal polynomials. Through the utilization of these operational matrices, the fractional-order problems can be transformed into a system of Sylvester-type matrix equations. This system is easily solvable using any computational software, thereby providing a practical framework for solving such equations. The results obtained are compared against various benchmarks, including an existing exact solution, Podlubny numerical techniques, analytical and numerical solvers, and reported solutions from stochastic techniques employing hybrid approaches. This comparative analysis serves to validate the accuracy of our proposed design scheme.

Accession Number: WOS:001193394700001

Author Identifiers:

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Riaz, Muhammad	ABA-9824-2021	
Agarwal, Praveen	I-7327-2012	
talib, imran		0000-0003-0115-4506

ISSN: 1658-3655

Record 124 of 274

Title: Minimal model of inelastic tunneling of vibrating magnetic molecules on superconducting substrates

Author(s): Koliogiorgos, A (Koliogiorgos, Athanasios); Korytar, R (Korytar, Richard)

Source: PHYSICAL REVIEW B **Volume:** 110 **Issue:** 23 **Article Number:** 235424 **DOI:** 10.1103/PhysRevB.110.235424 **Published Date:** 2024 DEC 20

Abstract: We present an efficient method of calculating the vibrational spectrum of a magnetic molecule adsorbed on a superconductor, directly related to the first derivative of the tunneling IV curve. The work is motivated by a recent scanning-tunneling spectroscopy of lead phthalocyanine on superconducting Pb(100), showing a wealth of vibrational excitations, the number of which highly exceeds molecular vibrations typically encountered on normal metals. We design a minimal model, which represents the

inelastic transitions by the spectral function of a frontier orbital of the molecule in isolation. The model allows for an exact solution; otherwise the full correlated superconducting problem would be hard to treat. The model parameters are supplied from an ab initio calculation, where the presence of the surface on the deformation of molecular geometry can be taken into account. The spectral function of the highest-occupied molecular orbital of the anionic PbPc1- shows the best agreement with the experimental reference among other molecular charge states and orbitals. The method allows us to include multiple vibrational transitions straightforwardly.

Accession Number: WOS:001389544900002

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Koliogiorgos, Athanasios	X-9318-2019	

ISSN: 2469-9950

eISSN: 2469-9969

Record 125 of 274

Title: Structural and magnetic properties of SmCrTiO5

Author(s): Susloparova, AE (Susloparova, Anna E.); Bolletta, JP (Bolletta, Juan Pablo); Kobzi, B (Kobzi, Balazs); Paecklar, AA (Paecklar, Arnold A.); Jouen, S (Jouen, Samuel); Fauth, F (Fauth, Francois); Nachbaur, V (Nachbaur, Virginie); Nassif, V (Nassif, Vivian); Suard, E (Suard, Emmanuelle); Sedmidubsky, D (Sedmidubsky, David); Kurbakov, AI (Kurbakov, Alexander I.); Maignan, A (Maignan, Antoine); Martin, C (Martin, Christine)

Source: PHYSICAL REVIEW B **Volume:** 110 **Issue:** 22 **Article Number:** 224429 **DOI:** 10.1103/PhysRevB.110.224429 **Published Date:** 2024 DEC 20

Abstract: We present results of a comprehensive experimental study of the compound SmCrTiO5, belonging to the RM2O5 family, where M is a mixture of two transition metals, Cr3+ and Ti4+. The studies were carried out using temperature-dependent synchrotron x-ray- and neutron-powder diffraction, and measuring the temperature- and field dependences of magnetization. No structural transition is observed between 2 and 450 K. The crystal structure of SmCrTiO5 is described in the orthorhombic space group Pbam. It is built from MO5 square pyramids and MO6 octahedra. The Sm3+ cations occupy a polyhedron of coordination 8, which shares edges with the two other polyhedra. Cr3+ and Ti4+ are found to differentially occupy each of the two transition-metal coordination sites, forming two substructures. Magnetic d3 Cr3+ ions occupy the octahedra which share edges to form chains, while nonmagnetic d0 Ti4+ ions occupy the pyramids. Magnetic susceptibility curves present a broad signal below 195 K with a maximum at about 100 K, characteristic of 1D antiferromagnetism. Nevertheless, long-range 3D magnetic order appears below 12 K as evidenced by neutron-powder diffraction. The refined magnetic structure is in addition supported by electronic structure calculations. From these data, a model of spin ordering in the ground state is proposed. Since the structural features are characteristic of alternating Heisenberg antiferromagnetic chains, the magnetic properties of SmCrTiO5 are compared with its SmCrGeO5 analog for which a spin gap was evidenced.

Accession Number: WOS:001389463600004

ISSN: 2469-9950

eISSN: 2469-9969

Record 126 of 274

Title: Comparison of non-synonymous/synonymous (dN/dS) ratios shows little evidence for a faster-Z effect in Furcifer chameleons after controlling for gene-specific evolutionary rates

Author(s): Andjel, L (Andjel, Lucija); Kratochvíl, L (Kratochvil, Lukas); Rovatsos, M (Rovatsos, Michail)

Source: JOURNAL OF HEREDITY **DOI:** 10.1093/jhered/esae070 **Early Access Date:** DEC 2024 **Published Date:** 2024 DEC 17

Abstract: The faster-X/Z effect hypothesis states that genes linked to X/Z chromosomes should accumulate mutations faster than autosomal genes. Although faster evolution of X/Z-linked genes has been reported in several plant and animal lineages, conflicting results have been reported in others. We examined the faster-Z effect in chameleons of the genus Furcifer, a lineage with differentiated ZZ/ZW chromosomes for at least 20 million yr. We sequenced the genomes of four species of Furcifer chameleons in the Illumina platform and compared the substitution rates of synonymous and non-synonymous mutations and their ratios among autosomal, Z-specific, and pseudoautosomal protein-coding genes. The inclusion of two chameleon outgroups lacking the differentiated ZZ/ZW sex chromosomes allowed us to control for gene-specific evolutionary rates that might confound the testing of the faster-X/Z effect. Significant differences in evolutionary rates were found between autosomal, Z-specific, and pseudoautosomal genes of Furcifer chameleons. However, the inclusion of the outgroups with different sex chromosomes suggests that these genes had different evolutionary rates prior to their incorporation into the differentiated ZZ/ZW sex chromosomes of the Furcifer genus. The results highlight the need to control for differences in the evolutionary rates of individual genes when testing for the faster-X/Z effect.

Accession Number: WOS:001379159600001

PubMed ID: 39575506

ISSN: 0022-1503

eISSN: 1465-7333

Record 127 of 274

Title: Impact of electron trapping on stimulated Raman scattering under incoherent broadband laser light in homogeneous plasma

Author(s): Blackman, DR (Blackman, David R.); Tikhonchuk, V (Tikhonchuk, Vladimir); Klimo, O (Klimo, Ondrej); Weber, S (Weber, Stefan)

Source: PHYSICAL REVIEW E **Volume:** 110 **Issue:** 6 **Article Number:** 065207 **DOI:** 10.1103/PhysRevE.110.065207 **Published Date:** 2024 DEC 16

Abstract: Backward stimulated Raman scattering is a three-wave coupling instability requiring the matching of an incoming pump light wave to a scattered light wave and an electron plasma wave. It can be harmful to laser-driven inertial confinement fusion because of the reflection of a part of the incident laser flux and the generation of suprathermal electrons that preheat the fuel. It is believed that by increasing the laser bandwidth, one can suppress the excitation of Raman scattering and mitigate its detrimental effects. It is demonstrated in this paper that using a broad bandwidth laser has little effect on stimulated Raman scattering in the kinetic inflation regime where Landau damping dominates, as the additional bandwidth allows the electron plasma wave to match a wider range of laser frequencies. As a result, plasma wave saturation and Raman backscattering levels remain high even when the laser bandwidth is much larger than the effective instability growth rate.

Accession Number: WOS:001391332700006

ISSN: 2470-0045

eISSN: 2470-0053

Record 128 of 274

Title: ²⁷Al NMR chemical shifts in zeolite MFI via machine learning acceleration of structure sampling and shift prediction

Author(s): Willimetz, D (Willimetz, Daniel); Erlebach, A (Erlebach, Andreas); Heard, CJ (Heard, Christopher J.); Grajciar, L (Grajciar, Lukas)

Source: DIGITAL DISCOVERY **Volume:** 4 **Issue:** 1 **Pages:** 275-288 **DOI:** 10.1039/d4dd00306c **Early Access Date:** DEC 2024 **Published Date:** 2025 JAN 15

Abstract: Zeolites, such as MFI, are versatile microporous aluminosilicate materials that are widely used in catalysis and adsorption processes. The location and the character of the aluminium within the zeolite framework is one of the important determinants of performance in industrial applications, and is typically probed by 27Al NMR spectroscopy. However, interpretation of 27Al NMR spectra is challenging, as first-principles computational modelling struggles to achieve the timescales and model complexity needed to provide reliable assignments. In this study, we deploy advanced machine learning-based methods to help bridge the time and model complexity scale by first utilizing neural network interatomic potentials to achieve significant speed-up in structure sampling compared to traditional density functional theory (DFT) approaches, and second by training regression models to cost-effectively predict the 27Al chemical shifts. This allows us, for the H-MFI zeolite as a use case, to comprehensively explore the effect of various conditions relevant to catalysis, including water loading, temperature, and the aluminium concentration, on the 27Al chemical shifts. We demonstrate that both water content and temperature significantly affect the chemical shift and do so in a non-trivial way that is highly T-site dependent, highlighting a need for adoption of realistic, case-specific models. We also observe that our approach is able to achieve close to quantitative agreement with relevant experimental data for such a complex zeolite as MFI, allowing for the tentative assignment of the experimental NMR peaks to specific T-sites. These findings provide a testament to the capabilities of machine learning approaches in providing reliable predictions of important spectroscopic observables for complex industrially relevant materials under realistic conditions.

Accession Number: WOS:001378563300001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Grajciar, Lukas	H-1266-2015	
Erlebach, Andreas	L-7200-2015	

eISSN: 2635-098X

Record 129 of 274

Title: Czech news dataset for semantic textual similarity

Author(s): Sido, J (Sido, Jakub); Seják, M (Sejak, Michal); Prazák, O (Prazak, Ondrej); Konopík, M (Konopik, Miloslav); Moravec, V (Moravec, Vaclav)

Source: LANGUAGE RESOURCES AND EVALUATION **DOI:** 10.1007/s10579-024-09795-z **Early Access Date:** DEC 2024 **Published Date:** 2024 DEC 7

Abstract: This paper describes a novel dataset consisting of sentences with two different semantic similarity annotations; with and without surrounding context. The data originate from the journalistic domain in the Czech language. The final dataset contains 138,556 human annotations divided into train and test sets. In total, 485 journalism students participated in the creation process. To increase the reliability of the test set, we compute the final annotations as an average of 9 individual annotation scores. We evaluate the dataset quality by measuring inter and intra-annotator agreements. Besides agreement numbers, we provide detailed statistics of the collected dataset. We conclude our paper with a baseline experiment of building a system for predicting the semantic similarity of sentences. Due to the massive number of training annotations (116,956), the model significantly outperforms an average annotator (0.92 versus 0.86 of Pearson's correlation coefficient).

Accession Number: WOS:001371498800001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sido, Jakub	AAL-5453-2020	
Moravec, Vaclav	JPK-8032-2023	
Konopik, Miloslav	AAR-6524-2020	

ISSN: 1574-020X
eISSN: 1574-0218

Record 130 of 274

Title: Estimating the Size and Composition of Customer Base Using Retail Transaction Data

Author(s): Sokol, O (Sokol, Ondrej); Holy, V (Holy, Vladimir)

Source: APPLIED STOCHASTIC MODELS IN BUSINESS AND INDUSTRY **DOI:** 10.1002/asmb.2914 **Early Access Date:** DEC 2024 **Published Date:** 2024 DEC 7

Abstract: The knowledge of the number of customers is the pillar of retail business analytics. In our setting, we assume that a portion of customers is monitored and easily counted due to the loyalty program while the rest is not monitored. The behavior of customers in both groups may significantly differ making the estimation of the number of unmonitored customers a nontrivial task. We identify shopping patterns of several customer segments which allows us to estimate the distribution of customers without the loyalty card using the maximum likelihood method. In a simulation study, we find that the proposed approach is quite precise even when the data sample is very small and its assumptions are violated to a certain degree. When a major violation is suspected, we suggest an interval approach. In an empirical study of a drugstore chain, we validate and illustrate the proposed approach in practice. The actual number of customers estimated by the proposed method is much higher than the number suggested by the naive estimate assuming the constant customer distribution. The proposed method can also be utilized to determine penetration of the loyalty program in the individual customer segments.

Accession Number: WOS:001374102600001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Holý, Vladimír	I-5814-2018	

ISSN: 1524-1904
eISSN: 1526-4025

Record 131 of 274

Title: Enhanced diffusion through multivalency

Author(s): Bartos, L (Bartos, Ladislav); Lund, M (Lund, Mikael); Vácha, R (Vacha, Robert)

Source: SOFT MATTER **Volume:** 21 **Issue:** 2 **DOI:** 10.1039/d4sm00778f **Early Access Date:** DEC 2024 **Published Date:** 2025 JAN 2

Abstract: The diffusion of macromolecules, nanoparticles, viruses, and bacteria is essential for targeting hosts or cellular destinations. While these entities can bind to receptors and ligands on host surfaces, the impact of multiple binding sites-referred to as multivalency-on diffusion along strands or surfaces is poorly understood. Through numerical simulations, we have discovered a significant acceleration in diffusion for particles with increasing valency, while maintaining the same overall affinity to the host surface. This acceleration arises from the redistribution of the binding affinity of the particle across multiple binding ligands. As a result, particles that are immobilized when monovalent can achieve near-unrestricted diffusion upon becoming multivalent. Additionally, we demonstrate that the diffusion of multivalent particles with a rigid ligand distribution can be modulated by patterned host receptors. These findings provide insights into the complex diffusion mechanisms of multivalent particles and biological entities, and offer new strategies for designing advanced nanoparticle systems with tailored diffusion properties, thereby enhancing their effectiveness in applications such as drug delivery and diagnostics.

Accession Number: WOS:001369389100001
PubMed ID: 39628400

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ISSN: 1744-683X

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Record 132 of 274

Title: A hairy giant among dwarves: Trichopelma grande, a distinct new species of tarantula from Cuba (Araneae: Theraphosidae)

Author(s): Ortiz, D (Ortiz, David); Fonseca, E (Fonseca, Elier)

Source: JOURNAL OF NATURAL HISTORY **Volume:** 58 **Issue:** 45-48 **Pages:** 2189-2205 **DOI:** 10.1080/00222933.2024.2401921 **Published Date:** 2024 DEC 1

Abstract: Large size, tropical climate, topographic complexity, and millions of years of isolation have turned the Greater Antillean islands into natural laboratories of evolution. Several groups have experienced explosive diversification across these islands, leading to highly diverse and endemic biotas and species experiencing unique adaptations. Here we describe a new tarantula species from the Vi ñales area, a biodiversity hotspot in western Cuba. Despite being a middle-sized species with large projected setae on the legs, reminiscent of those in arboreal tarantulas, phylogenomic analysis, diagnostic morphological features, and trap-door retreat building behaviour identifies it as the largest known representative of Trichopelma, and the only one with such hirsute legs. We provide mitochondrial barcoding data and a database of ultraconserved elements loci of the holotype of this species, which will help to include it in future phylogenetic studies of Theraphosidae. Given its limited distribution range, and its apparent absence in natural history collections despite its distinct appearance, this species might be scarce, positioning it as a potential conservation concern.http://www.zoobank.org/ urn:lsid:zoobank.org:pub:2F9ED7A1-1345-4295-A876-6B617ABF7C75

Accession Number: WOS:001355344100001

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ISSN: 0022-2933

eISSN: 1464-5262

Record 133 of 274

Title: Collimated beams of fast neutrons at the NPI CAS

Author(s): Ansorge, M (Ansorge, Martin); Majerle, M (Majerle, Mitja); Novák, J (Novak, Jan); Behal, R (Behal, Radek); Bém, P (Bem, Pavel); Koliadko, D (Koliadko, Daniil); Mrázek, J (Mrazek, Jaromir); Rataj, J (Rataj, Jan); Simecková, E (Simeckova, Eva); Stefánik, M (Stefanik, Milan); Stursa, J (Stursa, Jan); Yasin, Z (Yasin, Zafar)

Source: NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT **Volume:** 1071 **Article Number:** 170030 **DOI:** 10.1016/j.nima.2024.170030 **Early Access Date:** NOV 2024 **Published Date:** 2025 FEB

Abstract: The Nuclear Physics Institute of the Czech Academy of Sciences operates multiple neutron sources that can produce neutrons with energies up to 33 MeV. Recently, a segmented collimator was constructed to facilitate research on collimated beams of fast neutrons. In front of the collimator, anew quasi-monoenergetic neutron source was built using accelerated protons interacting with a 2.5 mm thick beryllium target. The collimated beam provides a neutron flux of approximately 106 n/cm2/s at the standard measurement position. To determine the parameters of the collimated neutron beam, various measurement techniques were employed, including scintillator-based time-of-flight mode, proton recoil telescope, and activation detection through the (n,2-3n) reaction on a yttrium sample. Furthermore,

Monte Carlo simulations were conducted to model the neutron transport through the collimator, and the results were subsequently compared to the experimental data obtained.

Accession Number: WOS:001362995800001

Author Identifiers:

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Majerle, Mitja	H-1030-2014	
Ansorge, Martin	D-1871-2018	

ISSN: 0168-9002

eISSN: 1872-9576

Record 134 of 274

Title: High spatial and spectral resolution dataset of hyperspectral look-up tables for 3.5 million traits and structural combinations of Central European temperate broadleaf forests

Author(s): Hanousek, T (Hanousek, Tomas); Slaninákova, T (Slaninakova, Terezia); Rebok, T (Rebok, Tomas); Janoutová, R (Janoutova, Ruzena)

Source: DATA IN BRIEF **Volume:** 57 **Article Number:** 111105 **DOI:** 10.1016/j.dib.2024.111105 **Early Access Date:** NOV 2024 **Published Date:** 2024 DEC

Abstract: Accurate retrieval of forest functional traits from remote sensing data is critical for monitoring forest health and productivity. To achieve sufficient accuracy using inverse methods it is essential to have representative database of simulated or measured spectral properties together with corresponding forest traits. However, existing datasets are often limited in scope, covering specific sites and times with simplified structures. This limitation hinders the development of generalizable machine learning models for trait prediction. To address this issue, we present a comprehensive highresolution dataset of hyperspectral Look-Up Tables (LUT) designed for Central European temperate broadleaf forests. The dataset includes 3.5 million unique combinations of leaf biochemical and canopy structural characteristics of forest scenes together with a variety of sun geometry. The spectral data cover wavelengths from 450 nm to 2300 nm, with a resolution of 2 nm. The dataset is organised into two files: one capturing the average reflectance of all scene pixels and another focusing solely on sunlit leaf pixels. LUT were generated using the Discrete Anisotropic Radiative Transfer model version 5.10.0. Virtual forest scenes were based on 3D tree European beech trees, adjusted to various leaf area index values and structural configurations to simulate natural forest variability. The reflectance data were processed using MATLAB and Python scripts, resulting in hyperspectral cubes that The dataset can be used to train machine learning models, such as Random Forest and Support Vector Machines, for predicting forest functional traits and assisting in the calibration of remote sensing algorithms. The biggest advantage of the dataset is high spectral and spatial resolution, together with the high number of different trait combinaThis is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/)

Accession Number: WOS:001359597600001

PubMed ID: 39624662

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Janoutova, Ruzena		0000-0003-1830-7556

ISSN: 2352-3409

Record 135 of 274

Title: Introduction of Phosphinine Ring into Aromatic Systems via Alkyne Cyclization

Author(s): Mizerová, E (Mizerova, Eliska); Kos, M (Kos, Martin); Jakubec, M (Jakubec, Martin); Pavlica, M (Pavlica, Marek); Zádny, J (Zadny, Jaroslav); Církva, V (Cirkva, Vladimir); Storch, J (Storch, Jan); Beránek, T (Beranek, Tomas)

Source: ADVANCED SYNTHESIS & CATALYSIS **DOI:** 10.1002/adsc.202401203 **Early Access Date:** NOV 2024 **Published Date:** 2024 NOV 13

Abstract: Recently developed synthetic protocols for the preparation of lambda 3-phosphanaphthalenes have broadened the general scope of organophosphorus chemistry, but a versatile protocol is still missing. Here, we describe a scalable synthetic approach for the construction of various substituted phosphanaphthalenes. We have obtained 11 derivatives through rigorous study and have demonstrated the robustness of this method. The optical properties of these phosphorus compounds and their aza and carbo analogues have been experimentally compared. Here, we show the power of the method in extending the synthesis to even larger polycyclic aromatic systems with embedded phosphine rings toward its potential applicability to materials science.

Accession Number: WOS:001357081500001

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ISSN: 1615-4150

eISSN: 1615-4169

Record 136 of 274

Title: Structural, Solvent, and Temperature Effects on Protein Junction Conductance

Author(s): Jonnalagadda, GN (Jonnalagadda, Gowtham Nirmal); Wu, XJ (Wu, Xiaojing); Hronek, L (Hronek, Lukas); Futera, Z (Futera, Zdenek)

Source: JOURNAL OF PHYSICAL CHEMISTRY LETTERS **Volume:** 15 **Issue:** 46 **Pages:** 11608-11614 **DOI:** 10.1021/acs.jpclett.4c02230 **Early Access Date:** NOV 2024 **Published Date:** 2024 NOV 12

Abstract: Cytochrome b 562 is a small redox-active heme protein that has served as an important model system for understanding biological electron transfer processes. Here, we present a comprehensive theoretical study of electron transport mechanisms in protein-metal junctions incorporating cytochrome b 562 using a multi-scale computational approach. Employing molecular dynamics (MD) simulations, we generated junction geometries for both vacuum-dried and solvated conditions, with the protein covalently bound to gold contacts in various configurations. Coherent tunneling, described by the Landauer-Buttiker formalism within the density functional theory (DFT) framework, is compared to the incoherent hopping charge transport mechanism captured by the semi-classical Marcus theory. The tunneling was identified as the dominant mechanism explaining the experimental data measured on the cytochrome b 562 junctions, exhibiting exponential yet very shallow distance dependence. While the structural orientations and protein contacts with the electrodes influence the junction conductance significantly, the solvation effects are relatively small, affecting the electronic properties mostly via the adsorption arrangement. On the other hand, the considerable temperature dependence of the conductance was found strong only for hopping, while the tunneling current magnitudes remain practically unaffected and are a good indicator of the coherent mechanism in this case.

Accession Number: WOS:001353288800001

PubMed ID: 39531285

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ISSN: 1948-7185

Record 137 of 274

Title: Fluorescence from a single-molecule probe directly attached to a plasmonic STM tip

Author(s): Friedrich, N (Friedrich, Niklas); Roslawska, A (Roslawska, Anna); Arrieta, X (Arrieta, Xabier); Kaiser, K (Kaiser, Katharina); Romeo, M (Romeo, Michelangelo); Le Moal, E (Le Moal, Eric); Scheurer, F (Scheurer, Fabrice); Aizpurua, J (Aizpurua, Javier); Borisov, AG (Borisov, Andrei G.); Neuman, T (Neuman, Tomas); Schull, G (Schull, Guillaume)

Source: NATURE COMMUNICATIONS **Volume:** 15 **Issue:** 1 **Article Number:** 9733 **DOI:** 10.1038/s41467-024-53707-2 **Published Date:** 2024 NOV 10

Abstract: The scanning tunneling microscope (STM) provides access to atomic-scale properties of a conductive sample. While single-molecule tip functionalization has become a standard procedure, fluorescent molecular probes remained absent from the available tool set. Here, the plasmonic tip of an STM is functionalized with a single fluorescent molecule and is scanned on a plasmonic substrate. The tunneling current flowing through the tip-molecule-substrate junction generates a narrow-line emission of light corresponding to the fluorescence of the negatively charged molecule suspended at the apex of the tip, i.e., the emission of the excited molecular anion. The fluorescence of this molecular probe is recorded for tip-substrate nanocavities featuring different plasmonic resonances, for different tip-substrate distances and applied bias voltages, and on different substrates. We demonstrate that the width of the emission peak can be used as a probe of the exciton-plasmon coupling strength and that the energy of the emitted photons is governed by the molecule interactions with its environment. Additionally, we theoretically elucidate why the direct contact of the suspended molecule with the metallic tip does not totally quench the radiative emission of the molecule.
Scanning tunneling microscopy (STM) gives access to the atomic-scale properties of matter. Here, the authors showcase the fluorescent functionalization of an STM tip using a single molecule in direct metal contact, permitting the local electrostatic and -dynamic environment to be probed.

Accession Number: WOS:001352879700004

PubMed ID: 39523359

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eISSN: 2041-1723

Record 138 of 274

Title: A unique symbiosome in an anaerobic single-celled eukaryote

Author(s): Jerlström-Hultqvist, J (Jerlstrom-Hultqvist, Jon); Gallot-Lavallée, L (Gallot-Lavallee, Lucie); Salas-Leiva, DE (Salas-Leiva, Dayana E.); Curtis, BA (Curtis, Bruce A.); Záhonová, K (Zahonova, Kristina); Cepicka, I (Cepicka, Ivan); Stairs, CW (Stairs, Courtney W.); Pipaliya, S (Pipaliya, Shweta); Dacks, JB (Dacks, Joel B.); Archibald, JM (Archibald, John M.); Roger, AJ (Roger, Andrew J.)

Source: NATURE COMMUNICATIONS **Volume:** 15 **Issue:** 1 **Article Number:** 9726 **DOI:** 10.1038/s41467-024-54102-7 **Published Date:** 2024 NOV 9

Abstract: Symbiotic relationships between eukaryotes and prokaryotes played pivotal roles in the evolution of life and drove the emergence of specialized symbiotic structures in animals, plants and fungi. The host-evolved symbiotic structures of microbial eukaryotes - the vast majority of such hosts in nature - remain largely unstudied. Here we describe highly structured symbiosomes within three free-living anaerobic protists (Anaeramoeba spp.). We dissect this symbiosis using complete genome sequencing and transcriptomics of host and symbiont cells coupled with fluorescence in situ hybridization, and 3D reconstruction using focused-ion-beam scanning electron microscopy. The emergence of the symbiosome is underpinned by expansion of gene families encoding regulators of membrane trafficking and phagosomal maturation and extensive bacteria-to-eukaryote lateral transfer. The symbionts reside deep within a symbiosomal membrane network that enables metabolic syntrophy by precisely positioning sulfate-reducing bacteria alongside host hydrogenosomes. Importantly, the symbionts maintain connections to the Anaeramoeba plasma membrane, blurring traditional boundaries between ecto- and endosymbiosis.
Symbiont-housing structures are well-studied in multicellular eukaryotes but rarely in unicellular protists. This study shows that low-oxygen-adapted Anaeramoebae have symbiosomes positioning sulfate-reducing bacteria near hydrogenosomes, with genomic analyses suggesting likely metabolic interactions.

Accession Number: WOS:001352369200019

PubMed ID: 39521804

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eISSN: 2041-1723

Record 139 of 274

Title: Endosome rupture enables enteroviruses from the family Picornaviridae to infect cells

Author(s): Ishemgulova, A (Ishemgulova, Aygul); Mukhamedova, L (Mukhamedova, Liya); Trebichalská, Z (Trebichalska, Zuzana); Rájecká, V (Rajecka, Veronika); Payne, P (Payne, Pavel); Smerdová, L (Smerdova, Lenka); Moravcová, J (Moravcova, Jana); Hrebik, D (Hrebik, Dominik); Buchta, D (Buchta, David); Skubnik, K (Skubnik, Karel); Füzik, T (Fuzik, Tibor); Vanácová, S (Vanacova, Stepanka); Novacek, J (Novacek, Jiri); Plevka, P (Plevka, Pavel)

Source: COMMUNICATIONS BIOLOGY **Volume:** 7 **Issue:** 1 **Article Number:** 1465 **DOI:** 10.1038/s42003-024-07147-9 **Published Date:** 2024 NOV 8

Abstract: Membrane penetration by non-enveloped viruses is diverse and generally not well understood. Enteroviruses, one of the largest groups of non-enveloped viruses, cause diseases ranging from the common cold to life-threatening encephalitis. Enteroviruses enter cells by receptor-mediated endocytosis. However, how enterovirus particles or RNA genomes cross the endosome membrane into the cytoplasm remains unknown. Here we used cryo-electron tomography of infected cells to show that endosomes containing enteroviruses deform, rupture, and release the virus particles into the cytoplasm. Blocking endosome acidification with bafilomycin A1 reduced the number of particles that released their genomes, but did not prevent them from reaching the cytoplasm. Inhibiting post-endocytic membrane remodeling with wiskostatin promoted abortive enterovirus genome release in endosomes. The rupture of endosomes also occurs in control cells and after the endocytosis of very low-density lipoprotein. In summary, our results show that cellular membrane remodeling disrupts enterovirus-containing endosomes and thus releases the virus particles into the cytoplasm to initiate infection. Since the studied enteroviruses employ different receptors for cell entry but are delivered into the cytoplasm by cell-mediated endosome disruption, it is likely that most if not all enteroviruses, and probably numerous other viruses from the

family Picornaviridae, can utilize endosome rupture to infect cells.
Enteroviruses from the family Picornaviridae enter cells by endocytosis. Subsequently, endosome rupture, induced by cell-mediated membrane remodeling, enables enteroviruses to reach the cell cytoplasm and initiate infection.

Accession Number: WOS:001351597600001

PubMed ID: 39511383

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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eISSN: 2399-3642

Record 140 of 274

Title: Shear Deformation of Non-modulated Ni₂MnGa Martensite: An Ab Initio Study

Author(s): Heczko, M (Heczko, Martin); Sesták, P (Sestak, Petr); Seiner, H (Seiner, Hanus); Zeleny, M (Zeleny, Martin)

Source: SHAPE MEMORY AND SUPERELASTICITY **Volume:** 10 **Issue:** 4 **Pages:** 474-486 **DOI:** 10.1007/s40830-024-00510-z **Early Access Date:** NOV 2024 **Published Date:** 2024 DEC

Abstract: The impact of shear deformation in (101)[101<overline>]\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$$(101)[10\overline{1}]$$\end{document} system of non-modulated (NM) martensite in Ni2MnGa ferromagnetic shape memory alloy is investigated by means of ab initio atomistic simulations. The shear system is associated with twinning of NM lattice and intermatensitic transformation to modulated structures. The stability of the NM lattice increases with increasing content of Mn. The most realistic shear mechanism for twin reorientation can be approximated by the simple shear mechanism, although the lowest barriers were calculated for pure shear mechanism. The energy barrier between twin variants further reduces due to spontaneous appearance of lattice modulation or, in other words, the nanotwins with thickness of two atomic planes. Such nanotwins appear also on the generalized planar fault energy (GPFE) curve calculated using a newly developed advanced procedure and exhibits even lower energy than the defect free NM structure. These nanotwin doublelayers are also basic building blocks of modulated structures and play an important role in intermartensitic transformation.

Accession Number: WOS:001349829700001

Author Identifiers:

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ISSN: 2199-384X

eISSN: 2199-3858

Record 141 of 274

Title: A simple approach to rotationally invariant machine learning of a vector quantity

Author(s): Martinka, J (Martinka, Jakub); Pederzoli, M (Pederzoli, Marek); Barbatti, M (Barbatti, Mario); Dral, PO (Dral, Pavlo O.); Pittner, J (Pittner, Jiri)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 161 **Issue:** 17 **Article Number:** 174104 **DOI:** 10.1063/5.0230176 **Published Date:** 2024 NOV 7

Abstract: Unlike with the energy, which is a scalar property, machine learning (ML) prediction of vector or tensor properties poses the additional challenge of achieving proper invariance (covariance) with

respect to molecular rotation. For the energy gradients needed in molecular dynamics (MD), this symmetry is automatically fulfilled when taking analytic derivative of the energy, which is a scalar invariant (using properly invariant molecular descriptors). However, if the properties cannot be obtained by differentiation, other appropriate methods should be applied to retain the covariance. Several approaches have been suggested to properly treat this issue. For nonadiabatic couplings and polarizabilities, for example, it was possible to construct virtual quantities from which the above tensorial properties are obtained by differentiation and thus guarantee the covariance. Another possible solution is to build the rotational equivariance into the design of a neural network employed in the model. Here, we propose a simpler alternative technique, which does not require construction of auxiliary properties or application of special equivariant ML techniques. We suggest a three-step approach, using the molecular tensor of inertia. In the first step, the molecule is rotated using the eigenvectors of this tensor to its principal axes. In the second step, the ML procedure predicts the vector property relative to this orientation, based on a training set where all vector properties were in this same coordinate system. As the third step, it remains to transform the ML estimate of the vector property back to the original orientation. This rotate-predict-rotate (RPR) procedure should thus guarantee proper covariance of a vector property and is trivially extensible also to tensors such as polarizability. The RPR procedure has an advantage that the accurate models can be trained very fast for thousands of molecular configurations, which might be beneficial where many training sets are required (e.g., in active learning). We have implemented the RPR technique, using the MLatom and Newton-X programs for ML and MD, and performed its assessment on the dipole moment along MD trajectories of 1,2-dichloroethane.

Accession Number: WOS:001346512600002

PubMed ID: 39484894

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Barbatti, Mario	F-5647-2014	0000-0001-9336-6607

ISSN: 0021-9606

eISSN: 1089-7690

Record 142 of 274

Title: Detection of Guanine Quadruplexes by Raman Optical Activity and Quantum-Chemical Interpretation of the Spectra

Author(s): Kkadan, MSP (Kkadan, Mohammed Siddhique Para); Jílek, S (Jilek, Stepan); Profant, V (Profant, Vaclav); Kapitán, J (Kapitan, Josef); Kessler, J (Kessler, Jiri); Bour, P (Bour, Petr)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 30 **Issue:** 70 **DOI:** 10.1002/chem.202403245 **Early Access Date:** NOV 2024 **Published Date:** 2024 DEC 13

Abstract: Quadruplexes formed by guanine derivatives or guanine-rich nucleic acids are involved in metabolism and genetic storage of many living organisms, they are used in DNA nanotechnologies or as biosensors. Since many quadruplex geometries are possible the determination of their structures in aqueous solutions is difficult. Raman optical activity (ROA) can make it easier: For guanosine monophosphate (GMP), we observed a distinct change of the spectra upon its condensation and quadruplex formation. The vibrational bands become more numerous, stronger, and narrower. In particular, a huge ROA signal appears below 200 cm-1. The aggregation can be induced by high concentration, low temperature, or by a metal ion. We focused on well-defined quadruplexes stabilized by potassium, where using molecular dynamics and density functional theory the spectra and particular features related to GMP geometric parameters could be understood. The simulations explain the main experimental trends and confirm that the ROA spectroscopy is sensitive to fine structural details, including guanine base twist in the quadruplex helix.

Accession Number: WOS:001354319600001

PubMed ID: 39329464

Author Identifiers:

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ISSN: 0947-6539

eISSN: 1521-3765

Record 143 of 274

Title: Molecular dynamics simulations unveil the aggregation patterns and salting out of polyarginines at zwitterionic POPC bilayers in solutions of various ionic strengths

Author(s): Nguyen, MTH (Nguyen, Man Thi Hong); Vazdar, M (Vazdar, Mario)

Source: COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL **Volume:** 23 **Pages:** 3897-3905 **DOI:** 10.1016/j.csbj.2024.11.004 **Early Access Date:** NOV 2024 **Published Date:** 2024 DEC

Abstract: This study employs molecular dynamics (MD) simulations to investigate the adsorption and aggregation behavior of simple polyarginine cell-penetrating peptides (CPPs), specifically modeled as R9 peptides, at zwitterionic phosphocholine POPC membranes under varying ionic strengths of two peptide concentrations and two concentrations of NaCl and CaCl2. The results reveal an intriguing phenomenon of R9 aggregation at the membrane, which is dependent on the ionic strength, indicating a salting-out effect. As the peptide concentration and ionic strength increase, peptide aggregation also increases, with aggregate lifetimes and sizes showing a corresponding rise, accompanied by the total decrease of adsorbed peptides at the membrane surface. Notably, in high ionic strength environments, large R9 aggregates, such as octamers, are also observed occasionally. The salting-out, typically uncommon for short positively charged peptides, is attributed to the unique properties of arginine amino acid, specifically by its side chain containing amphiphilic guanidinium (Gdm+) ion which makes both intermolecular hydrophobic like-charge Gdm+ - Gdm+ and salt-bridge Gdm+ - C-terminus interactions, where the former are increased with the ionic strength, and the latter decreased due to electrostatic screening. The aggregation behavior of R9 peptides at membranes can also be linked to their CPP translocation properties, suggesting that aggregation may aid in translocation across cellular membranes.

Accession Number: WOS:001361756500001

PubMed ID: 39559777

Author Identifiers:

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Vazdar, Mario	T-4589-2019	

ISSN: 2001-0370

Record 144 of 274

Title: Atomically resolved imaging of the conformations and adsorption geometries of individual β-cyclodextrins with non-contact AFM

Author(s): Grabarics, M (Grabarics, Marko); Mallada, B (Mallada, Benjamin); Edalatmanesh, S (Edalatmanesh, Shayan); Jiménez-Martín, A (Jimenez-Martin, Alejandro); Pykal, M (Pykal, Martin); Ondrácek, M (Ondracek, Martin); Kuehrova, P (Kuehrova, Petra); Struwe, WB (Struwe, Weston B.); Banás, P (Banas, Pavel); Rauschenbach, S (Rauschenbach, Stephan); Jelínek, P (Jelinek, Pavel); de la Torre, B (de la Torre, Bruno)

Source: NATURE COMMUNICATIONS **Volume:** 15 **Issue:** 1 **Article Number:** 9482 **DOI:** 10.1038/s41467-024-53555-0 **Published Date:** 2024 NOV 2

Abstract: Glycans, consisting of covalently linked sugar units, are a major class of biopolymers essential to all known living organisms. To better understand their biological functions and further applications in fields from biomedicine to materials science, detailed knowledge of their structure is essential. However, due to the extraordinary complexity and conformational flexibility of glycans, state-of-the-art glycan analysis methods often fail to provide structural information with atomic precision. Here, we combine electrospray deposition in ultra-high vacuum with non-contact atomic force microscopy and theoretical calculations to unravel the structure of beta-cyclodextrin, a cyclic glucose oligomer, with atomic-scale detail. Our results, established on the single-molecule level, reveal the different adsorption geometries and conformations of beta-cyclodextrin. The position of individual hydroxy groups and the location of the stabilizing intramolecular H-bonds are deduced from atomically resolved images, enabling the unambiguous assignment of the molecular structure and demonstrating the potential of the method for glycan analysis.
Glycans are structurally complex biomolecules and very challenging to analyse. Here the authors show atomically resolved imaging of beta-cyclodextrins with non-contact atomic force microscopy, revealing the structure of individual glycans with atomic detail.

Accession Number: WOS:001346923200021

PubMed ID: 39488518

Author Identifiers:

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Ondráček, Martin	A-1871-2012	
De la Torre, Bruno	R-4536-2019	
Edalatmanesh, Shayan	KHZ-1711-2024	

eISSN: 2041-1723

Record 145 of 274

Title: Tm@C₈₂: Calculated Isomeric Populations

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

Source: ECS JOURNAL OF SOLID STATE SCIENCE AND TECHNOLOGY **Volume:** 13 **Issue:** 11 **Article Number:** 111002 **DOI:** 10.1149/2162-8777/ad910e **Published Date:** 2024 NOV 1

Abstract: Relative equilibrium populations of the four potential-energy-lowest IPR (isolated-pentagon-rule) isomers of Tm@C-82 under high synthetic temperatures are calculated using the Gibbs energy based on molecular characteristics from the density functional theory calculations at the B3LYP/6-31G*similar to SDD level. Tm@C-2v(9)-C-82 and Tm@C-s(6)-C-82 are concluded as the most populated species. The calculations agree with available observations.

Accession Number: WOS:001363849900001

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Record 146 of 274

Title: Genome-Wide Data Uncover Cryptic Diversity With Multiple Reticulation Events in the Balkan-Anatolian Cardamine (Brassicaceae) Species Complex

Author(s): Slenker, M (Slenker, Marek); Kantor, A (Kantor, Adam); Senko, D (Senko, Dusan); Mártonfiová, L (Martonfiova, Lenka); Srámková, G (Sramkova, Gabriela); Cetlová, V (Cetlova, Veronika); Dönmez, AA (Donmez, Ali A.); Yüzbasioglu, S (Yuzbasioglu, Sirri); Zozomová-Lihová, J (Zozomova-Lihova, Judita)

Source: MOLECULAR ECOLOGY **Volume:** 33 **Issue:** 22 **DOI:** 10.1111/mec.17564 **Early Access Date:** OCT 2024 **Published Date:** 2024 NOV

Abstract: Plant species diversity may be considerably underestimated, especially in evolutionarily complex genera and in diversity hotspots that have enabled long-term species persistence and diversification, such as the Balkan Peninsula. Here, we address the topic of underexplored plant diversity and underlying evolutionary and biogeographic processes by investigating the hygrophytic mountain species complex of Cardamine acris s.l. distributed in the Balkans (three subspecies within C. acris) and northwestern Anatolia (C. anatolica). We performed a series of phylogenetic and phylogeographic analyses based on restriction-site associated DNA sequencing (RADseq) and target enrichment (Hyb-Seq) data in combination with habitat suitability modelling. We found C. anatolica as a clade nested within the Balkan C. acris, probably resulting from a founder event, and uncovered three allopatric cryptic lineages within C. acris subsp. acris, allowing us to recognise a total of six entities in this complex. We observed the deepest genetic split within C. acris subsp. acris in the western Balkans, which was at odds with taxonomy and showed no distribution gap. We inferred vicariance as the most likely process for population divergence in the Balkans, accompanied by gene flow between the recognised entities, which was consistent with the modelled habitat suitability dynamics. Furthermore, we discovered several polyploid populations in C. acris, representing both pure intra- and inter-lineage hybrid polyploids, but detected only minor traces of hybridization with related congeners. Overall, our results illustrate that diverse evolutionary processes may influence the history of mountain plant species in the Balkan Peninsula, including vicariance, reticulation, polyploidization and cryptic diversification.

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Record 147 of 274

Title: Revealing the effect of host-guest complementarity in supramolecular monofunctional platinum(<sc>ii</sc>) drugs

Author(s): Paul, SS (Paul, Shib Shankar); Novotny, J (Novotny, Jan); Jakubec, J (Jakubec, Jakub); Petrláková, K (Petrlakova, Katerina); Jurcek, P (Jurcek, Pia); Rasková, K (Raskova, Klara); Kuchynka, M (Kuchynka, Michaela); Masarík, M (Masarik, Michal); Kulhánek, P (Kulhanek, Petr); Marek, R (Marek, Radek)

Source: INORGANIC CHEMISTRY FRONTIERS **Volume:** 11 **Issue:** 23 **Pages:** 8510-8525 **DOI:** 10.1039/d4qi02012j **Early Access Date:** OCT 2024 **Published Date:** 2024 NOV 19

Abstract: Monofunctional platinum(ii) compounds bearing planar aromatic ligands can be significantly more potent for the treatment of tumors than the traditional bifunctional platinum(ii) systems derived from cisplatin. Their properties can be modulated by using a drug carrier, for example, by trapping them into a macrocyclic cavitand and releasing the metallodrug in a controlled manner. In this work, we introduce new monofunctional platinum(ii) compounds with the general structure cis-[PtII(NH3)2Cl(4-R-py)]+NO3- as direct analogs of pyriplatin, cis-[PtII(NH3)2Cl(py)]+. We investigated their chemical activation by aquation in host-guest (HG) complexes with the cucurbit[7]uril (CB7) macrocycle. We used a range of NMR techniques to characterize the HG complexation in detail, and the effects of the ligand on the structure and aquation of chloride at the platinum center in the HG complexes were rationalized with the support of molecular dynamics (MD) simulations and density-functional theory (DFT) calculations. Biological screening of the cytotoxicity and the drug uptake by cell lines A2780 and A2780/CP showed that the cytotoxicity of the Pt-compound with 4-phenylpyridine and 4-pentafluorophenylpyridine ligand was comparable to that of cisplatin and that the cytotoxicity and drug uptake of the Pt-compound with a 4-(1-adamantyl)pyridine ligand was greatly modulated by the CB7 carrier. Our observations indicate great potential for HG complexes in the future supramolecular design and structural tailoring of biological activity.

Accession Number: WOS:001344416300001

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ISSN: 2052-1553

Record 148 of 274

Title: Ageing and dynamics of the tailed radio galaxies in Abell 2142

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Source: ASTRONOMY & ASTROPHYSICS **Volume:** 690 **Article Number:** A329 **DOI:** 10.1051/0004-6361/202451515 **Published Date:** 2024 OCT 22

Abstract: Context. Tailed radio galaxies are shaped by ram pressure that is due to the high-velocity motion of their host through the intracluster medium (ICM). Recent works have reported on the increasing complexity of the phenomenology of tailed galaxies, with departures from theoretical ageing models and novel evidence of re-energising mechanisms that are nonetheless unclear. Aims. The nearby (z = 0.0894) galaxy cluster Abell 2142 hosts two tailed galaxies, namely T1 and T2, which exhibit peculiar morphological features. We aim to investigate the properties of T1 and T2 and constrain their spectral evolution, dynamics, and interactions with the ICM. Methods. We combined data from LOw Frequency Array (LOFAR), upgraded Giant Metrewave Radio Telescope (uGMRT), Very Large Array (VLA), and MeerKAT (from 30 MHz to 6.5 GHz) to carry out a detailed spectral analysis of T1 and T2. We analysed the surface brightness profiles, measured integrated and spatially resolved spectral indices. We performed a comparison with single injection ageing models. The Chandra X-ray data were used to

search for discontinuities in the ICM properties in the direction of the targets. Results. The spectral properties of T1 at low frequencies can be predicted by ageing models and provide constraints on the 3D dynamics of the host by assuming a constant velocity. However, a more complex scenario is suggested by the sharp transitions along sub-regions of the tail, local surface brightness enhancements, and a spectral shape at high frequencies that is not predicted by any of the models. This scenario may plausibly involve hydrodynamical instabilities and particle mixing. T2 exhibits unusual morphological and surface brightness features, and its spectral behaviour is not predicted by standard models. The effects of two active galactic nucleus (AGN) outburst events during the infall of T2 towards the cluster centre could potentially explain its characteristic properties.

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Record 149 of 274

Title: Haemoglobin Gene Repertoire in Teleost and Cichlid Fishes Shaped by Gene Duplications and Genome Rearrangements

Author(s): Omelchenko, D (Omelchenko, Dmytro); Bitja-Nyom, AR (Bitja-Nyom, Arnold Roger); Matschiner, M (Matschiner, Michael); Malinsky, M (Malinsky, Milan); Indermaur, A (Indermaur, Adrian); Salzburger, W (Salzburger, Walter); Bartos, O (Bartos, Oldrich); Musilova, Z (Musilova, Zuzana)

Source: MOLECULAR ECOLOGY **Volume:** 33 **Issue:** 22 **DOI:** 10.1111/mec.17559 **Early Access Date:** OCT 2024 **Published Date:** 2024 NOV

Abstract: Haemoglobin is a key molecule for oxygen transport in vertebrates. It exhibits remarkable gene diversity in teleost fishes, reflecting adaptation to various aquatic environments. In this study, we present the dynamic evolution of haemoglobin subunit genes based on a comparison of high-quality genome assemblies of 24 vertebrate species, including 17 teleosts (of which six are cichlids). Our findings indicate that teleost genomes contain a range of haemoglobin genes, from as few as five in fugu to as many as 43 in salmon, with the latter being the largest repertoire found in vertebrates. We find evidence that the teleost ancestor had at least four Hb alpha and three or four Hb beta subunit genes, and that the current gene diversity emerged during teleost radiation, driven primarily by (tandem) gene duplications, genome compaction, and rearrangement dynamics. We provide insights into the genomic organisation of haemoglobin clusters in different teleost species. We further show that the evolution of paralogous rhbdf1 genes flanking both teleost clusters (LA and MN) supports the hypothesis for the origin of the LA cluster by rearrangement within teleosts, rather than by the teleost specific whole-genome duplication. We specifically focus on cichlid fishes, where adaptation to low oxygen environment plays role in species diversification. Our analysis of six cichlid genomes, including Pungu maclareni from the Barombi Mbo crater lake, for which we sequenced a representative genome, reveals 18-32 copies of the Hb genes, and elevated rates of non-synonymous substitutions compared to other teleosts. Overall, this work facilitates a deeper understanding of how haemoglobin genes contribute to the adaptive potential of teleosts.

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PubMed ID: 39435681

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Record 150 of 274

Title: Design rules for doped transition metal dichalcogenides heterostructures

Author(s): Perviz, E (Perviz, Elliot); Cammarata, A (Cammarata, Antonio); Polcar, T (Polcar, Tomas)

Source: PHYSICAL REVIEW MATERIALS **Volume:** 8 **Issue:** 10 **Article Number:** 106001 **DOI:** 10.1103/PhysRevMaterials.8.106001 **Published Date:** 2024 OCT 22

Abstract: Transition metal dichalcogenides (TMDs) are the base materials for diverse technological devices such as memory devices, and nanotribological systems. Their flexible MX2 stoichiometry enables the fine-tuning of their properties via cation or anion substitution, thus allowing heterostructures with diverse functionalities to be engineered at the nanoscale. In this respect, we perform first-principles simulations to individuate possible novel structures derived from monolayer and bilayer MoS2 and WS2 alloyed with various metal and nonmetal dopants at different concentrations. We evaluate the relative stability and characterize the mechanisms responsible for their formation through electronic descriptors. Specifically, we identify bond covalency and orbital polarization as collective indicators for favorable electronic distributions, while the electronic structure of the isolated atom may be used for the selection of suitable dopants. The proposed methodology constitutes a general protocol, which can easily be extended to van der Waals heterostructures beyond those based on TMDs. Finally, the methodology can be used to help machine learning algorithms screen material databases for high-throughput discovery of new van der Waals-based alloys.

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Record 151 of 274

Title: Enhancing the radiation- and oxidation-resistance of Cr-based coatings via structure regulation and composition optimization

Author(s): Wang, RD (Wang, Renda); Daghbouj, N (Daghbouj, Nabil); Yu, P (Yu, Ping); Li, P (Li, Peng); Meng, FP (Meng, Fanping); Cammarata, A (Cammarata, Antonio); Li, BS (Li, Bingsheng); Polcar, T (Polcar, Tomas); Babor, P (Babor, P.); Huang, Q (Huang, Qing); Ge, FF (Ge, Fangfang)

Source: JOURNAL OF MATERIALS SCIENCE & TECHNOLOGY **Volume:** 218 **Pages:** 153-169 **DOI:** 10.1016/j.jmst.2024.08.051 **Early Access Date:** OCT 2024 **Published Date:** 2025 MAY 20

Abstract: Cr coatings, as protective coatings of Zr-alloy fuel claddings, inevitably suffer from irradiation damage before they would possibly run into the accident condition. This study evaluates the radiation and oxidation tolerance of three Cr-based coatings with different microstructures (Cr, CrAlSi, and CrAlSiN) through He2 + ion irradiation and 1200 degrees C steam oxidation. The Cr and CrAlSi coatings experienced significant structural degradation, characterized by He bubble aggregation and amplified Kirkendall effects at elevated temperatures. In contrast, the irradiated CrAlSiN coating maintained structural integrity without measurable irradiation hardening. Following annealing at 800 degrees C for 30 min, approximately 40 % of injected He atoms were released, indicating a "self-healing" mechanism. The mechanism is attributed to uniformly distributed, low-density channels that act as sinks and release paths for irradiation-induced defects. Density functional theory simulations suggest that N atoms promote significant rearrangement of ions surrounding the free volume, inhibiting the formation of sites capable of trapping He atoms. Moreover, the CrAlSiN coating exhibited superior oxidation resistance compared to the Cr and CrAlSi coatings, even under high-temperature steam conditions. Notably, the irradiated CrAlSiN sample displayed a significantly thinner oxide scale compared to the pristine one (almost half), owing to a more protective oxide scale and rapid outward diffusion of Cr, Al, and Si through nanochannel veins. These findings illuminate the effects of structure and composition on irradiation and oxidation behavior in Cr-based coatings, offering insights for developing new-generation accident-tolerance fuel coatings for Zr-alloy claddings. (c) 2024 Published by Elsevier Ltd on behalf of The editorial office of Journal of Materials Science & Technology.

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Record 152 of 274

Title: Storage and retrieval of von Neumann measurements via indefinite causal order structures

Author(s): Lewandowska, P (Lewandowska, Paulina); Kukulski, R (Kukulski, Ryszard)

Source: PHYSICAL REVIEW A **Volume:** 110 **Issue:** 4 **Article Number:** 042422 **DOI:** 10.1103/PhysRevA.110.042422 **Published Date:** 2024 OCT 18

Abstract: This work presents the problem of learning an unknown von Neumann measurement of dimension d using indefinite causal structures. In the considered scenario, we have access to N copies of the measurement. We use the formalism of process matrices to store information about the given measurement that later will be used to reproduce its best possible approximation. Our goal is to compute the maximum value of the average fidelity function Fd (N) of our procedure. We prove that Fd (N) = 1 - O (N 1 2) for arbitrary but fixed dimension d . Furthermore, we present the SDP program (semi-definite program) for computing F d (N). Basing on the numerical investigation, we show that for the qubit von Neumann measurements using indefinite causal learning structures provide better approximation than quantum networks, starting from N 3.

Accession Number: WOS:001340811100002

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Record 153 of 274

Title: Persistence Over Millennia Through Extreme Clonal Longevity: Phylogenomic Insight Into History of One of the World's Rarest Plant Species

Author(s): Mráz, P (Mraz, Patrik); Flasková, L (Flaskova, Lenka); Chrtek, J (Chrtek, Jindrich); Mrázová, V (Mrazova, Viera); Puscas, M (Puscas, Mihai); Josefiová, J (Josefiova, Jirina); Záveská, E (Zaveska, Eliska)

Source: JOURNAL OF BIOGEOGRAPHY **Volume:** 52 **Issue:** 1 **Pages:** 199-212 **DOI:** 10.1111/jbi.15028 **Early Access Date:** OCT 2024 **Published Date:** 2025 JAN

Abstract: AimThe evolutionary history of European alpine plant species with medium to large geographical ranges is relatively well explored. Here, we investigate the genetic structure and diversity of an extremely narrow endemic and one of the world's rarest plants.LocationEastern Carpathians, Romania.TaxonAndryala laevitomentosa (Asteraceae), an evolutionarily isolated herb species with a worldwide range limited to five micropopulations distributed along a 1.8 km long mountain ridge.MethodsWe used three plastid loci, nuclear ribosomal ITS and genome-wide, mostly nuclear 26,272 Single-Nucleotide Polymorphism (SNPs) obtained from RAD-seq data. We assessed haplotype and genotype diversity, dated the resulting phylogeographic structure, quantified seed production and inferred vegetative propagation.ResultsMaternally inherited plastid markers and nuclear genomic data revealed a concordant pattern: (i) limited genetic diversity, with seven cpDNA haplotypes and 11 RAD-seq multilocus genotypes; (ii) a strong geographic structure corresponding to spatially isolated genets (clones). The species is likely of early Pleistocene origin (c. 2 Mya), and the estimated age of individual clones varied from c. 24 to 64 Kya. The average seed set assessed over 3 years was only 0.4%. However, the species reproduces veg by axillary and adventitious rosettes formed on rhizomes and roots, respectively.Main ConclusionsThe strong trade-off between sexual and vegetative reproduction explains not only a deep and ancient phylogeographic structure but also the rarity of the species. Its survival depends almost entirely on vegetative reproduction. The genets of A. laevitomentosa are amongst the oldest clones ever documented in angiosperms. The persistence of these clones in situ for tens of thousands of years suggests an exceptional ability of this species to adapt to major climatic oscillations throughout the Pleistocene and Holocene and challenge our perception of the extent of resilience in plants.

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Author	Web of Science ResearcherID	ORCID Number
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Record 154 of 274

Title: Enhancing Extraction and Suppressing Cooling of Hot Electrons in Lead Halide Perovskites by Dipolar Surface Passivation

Author(s): Zhou, ZB (Zhou, Zhaobo); Wu, Y (Wu, Yang); He, JJ (He, Junjie); Frauenheim, T (Frauenheim, Thomas); Prezhdo, OV (Prezhdo, Oleg V.)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **Volume:** 146 **Issue:** 43 **Pages:** 29905-29912 **DOI:** 10.1021/jacs.4c12042 **Early Access Date:** OCT 2024 **Published Date:** 2024 OCT 17

Abstract: Slowing hot carrier (HC) cooling and improving HC extraction are considered two pivotal factors for enhancing power conversion efficiency in emerging HC photovoltaic applications of

perovskites and other materials. Employing ab initio quantum dynamics simulations, we demonstrate the simultaneous slow cooling and efficient extraction of hot electrons at the C-60/CsPbI3 interface through dipolar surface passivation with phenethylammonium and 4-fluorophenethylammonium ligands. The passivation effectively suppresses I-Pb lattice vibrations, weakens the hot electron-phonon interaction in CsPbI3, and thus slows down the HC cooling. At the same time, the dipolar surface passivation elevates the LUMO + 1 state in C-60 and reduces the energy gap for HC extraction. Concurrently, higher-frequency vibrations of the dipolar layer enhance the coupling between C-60 and CsPbI3, promoting efficient HC extraction further. These phenomena are intensified with increased polarity of the dipolar layer. Furthermore, we find that dipolar passivation has the opposite influence on cold electron collection at the band edge, underscoring the fact that the observed improvement in photovoltaic performance stems preferentially from the effective utilization of HCs rather than cold electrons. The work provides a new strategy for achieving high-performance HC perovskite solar cells.

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Record 155 of 274

Title: Exceptional stability of the sugammadex-solasodine complex: Insights from experimental and theoretical studies

Author(s): Kalydi, E (Kalydi, Eszter); Sebák, F (Sebak, Fanni); Fiser, B (Fiser, Bela); Minofar, B (Minofar, Babak); Moussong, E (Moussong, Eva); Malanga, M (Malanga, Milo); Bodor, A (Bodor, Andrea); Kardos, J (Kardos, Jozsef); Béni, S (Beni, Szabolcs)

Source: CARBOHYDRATE POLYMERS **Volume:** 348 **Article Number:** 122819 **DOI:** 10.1016/j.carbpol.2024.122819 **Early Access Date:** OCT 2024 **Published Date:** 2025 JAN 15 **Part:** A

Abstract: Sugammadex (SGM) is the first cyclodextrin (CD)-based selective relaxant binding agent. We investigated its ability to capture natural aminosteroid phytotoxins, and assessed its potential as an antidote for intoxication. Solasodine (SS), a toxic alkaloid from the Solanaceae family, was chosen as the model compound. Complexation was studied using nuclear magnetic resonance (NMR) spectroscopy, molecular modelling, and isothermal titration calorimetry (ITC). NMR in various D2O/DMSO-d6 media revealed a particularly stable inclusion-type complex, identifying a slow exchange process between the CD and the aminosteroid along with a less significant fast exchange between DMSO and SGM. Using various NMR techniques, the structure and kinetic/thermodynamic parameters of the inclusion complex were explored. Theoretical calculations showed the secondary amino head of SS near the carboxylate ends of the SGM sidechains, facilitating intermolecular ionic interactions. ITC experiments in an aqueous environment provided Ka stability constants of 7.03 x 106 M- 1 and 4.17 x 106 M- 1 at 25 degrees C and 37 degrees C, respectively, similar to previously reported SGM complexes with aminosteroid neuromuscular blockers. Finally, SGM significantly increased cell survival and reduced SS toxicity in mHippoE-14 mouse hippocampal embryonic cells, supporting the hypothesis that SGM could act as an antidote to SS's toxic effects.

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PubMed ID: 39562094

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Record 156 of 274

Title: Boosting Enzyme Activity in Biomass Conversion by Modulating the Hydrolysis Process of Cellobiohydrolases

Author(s): Liu, H (Liu, Han); Ding, Y (Ding, Yu); Mazurkewich, S (Mazurkewich, Scott); Pei, WW (Pei, Wenwen); Wei, XX (Wei, Xiuxin); Larsbrink, J (Larsbrink, Johan); Chipot, C (Chipot, Christophe); Hong, ZY (Hong, Zhangyong); Cai, WS (Cai, Wensheng); Zong, ZY (Zong, Zhiyou)

Source: ACS CATALYSIS **Volume:** 14 **Issue:** 21 **Pages:** 16044-16054 **DOI:** 10.1021/acscatal.4c05393 **Early Access Date:** OCT 2024 **Published Date:** 2024 OCT 16

Abstract: Cellobiohydrolases (CBHs) are the most significant cellulose-degrading enzymes, the performance of which determines the cost-effective utilization of renewable lignocellulosic resources. Most engineering strategies for improving CBH hydrolysis are currently focused on accelerating the noncatalytic enzyme-substrate dissociation by increasing the flexibility of eight substrate-enclosing loops (SELs), which does not take the catalysis into account or even deteriorates it. Here, in the model Trichoderma reesei CBHI, we identified a key SEL that affects the dissociation by examining enzyme-enzyme/substrate interactions. Furthermore, through analyzing the hydrogen-bonding network for the catalytic region, we detected a crucial residue D262. Root-mean-square-fluctuation analysis indicates that its replacement with valine (D262V) markedly improves the stability of the catalytic triad. Through QM/MM simulations, we determined that this mutation diminished the free-energy barrier against catalysis by 2.3 kcal/mol and increased k(cat) by 53.1%, as determined in kinetic experiments. Additionally, the substitution caused a significant enhancement of SEL flexibility and led to a lowered dissociation barrier by 2.1 kcal/mol. The cellobiose yield was increased by 49.8%, owing to the impact of the single valine replacement on the enzyme hydrolysis. This work unlocks a brand-new engineering direction for industrially important CBHs, contributing to more efficient depolymerization of renewable lignocellulose.

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ISSN: 2155-5435

Record 157 of 274

Title: The Hydrogen-Bond Continuum in the Salt/Cocrystal Systems of Quinoline and Chloro-Nitrobenzoic Acids

Author(s): Stocek, JR (Stocek, Jakub Radek); Blahut, J (Blahut, Jan); Chalupná, S (Chalupna, Simona); Cejka, J (Cejka, Jan); Stepánová, S (Stepanova, Sille); Kasicka, V (Kasicka, Vaclav); Husák, M (Husak, Michal); Dracínsky, M (Dracinsky, Martin)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 30 **Issue:** 68 **DOI:** 10.1002/chem.202402946 **Early Access Date:** OCT 2024 **Published Date:** 2024 DEC 5

Abstract: This study investigates the hydrogen-bond geometry in six two-component solid systems composed of quinoline and chloro-nitrobenzoic acids. New X-ray diffraction studies were conducted using both the conventional independent-atom model and the more recent Hirshfeld atom-refinement method, with the latter providing precise hydrogen-atom positions. The systems can be divided into salts (the hydrogen atom transferred to the quinoline nitrogen), cocrystals (the hydrogen atom retained by the acid), and intermediate structures. Solid-state NMR experiments corroborated the X-ray diffraction-derived H-N distances. DFT calculations, using five functionals including hybrid B3LYP and PBE0, showed varying energy profiles for the hydrogen bonds, with notable differences across functionals. These calculations revealed different preferences for salt or cocrystal structures, depending on the functional used. Path-integral molecular dynamics simulations incorporating nuclear quantum effects demonstrated significant hydrogen-atom delocalization, forming a hydrogen-bond continuum, and provided average N-H distances in excellent agreement with experimental results. This comprehensive experimental and theoretical approach highlights the complexity of multicomponent solids. The study emphasizes that the classification into salts or cocrystals is frequently inadequate, as the hydrogen atom is often significantly delocalized in the hydrogen bond. This insight is crucial for understanding and predicting the behavior of such systems in pharmaceutical applications.
Hydrogen-bond continuum in six two-component solid systems is investigated using a complex experimental and computational methodology consisting of X-ray diffraction experiments with Hirshfeld atom-refinement, solid-state NMR spectroscopy and DFT calculations. Path-integral molecular dynamics simulations incorporating nuclear quantum effects demonstrated significant hydrogen-atom delocalization and provided average N-H distances in excellent agreement with experimental results.
image

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Dracinsky, Martin	B-5813-2013	0000-0002-4495-0070

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Record 158 of 274

Title: Interface-mediated sp 2- sp 3 interconversion in ultrahard diamond-graphite nanocomposites with supertoughness

Author(s): Xu, TF (Xu, Tengfei); Liu, ZR (Liu, Zhaorui); Legut, D (Legut, Dominik); Zhang, RF (Zhang, Ruifeng)

Source: PHYSICAL REVIEW B **Volume:** 110 **Issue:** 13 **Article Number:** 134107 **DOI:** 10.1103/PhysRevB.110.134107 **Published Date:** 2024 OCT 16

Abstract: Recently synthesized diamond-graphite nanocomposites, consisting of diamond and graphite nanodomains interlocked via coherent interfaces (termed gradia), exhibit an impressive combination of ultrahigh hardness and superior toughness [Luo et al., Nature (London) 607, 486 (2022)]. This extraordinary finding challenges the prevailing understanding of the widespread trade-off relationship in strong covalent solids, while the toughening mechanism of gradia remains mysterious. Here, we unveil an sp 2- sp 3 interconversion mechanism, where the graphitization or the bond failures are effectively suppressed through layer-by-layer migration of the interfaces towards diamond (or graphite) domains, which originates from the sequential metallization starting from the diamond atomic layers adjacent to the interface with weakened sp 3 hybridization and the associated inverse process, i.e., metal-semiconductor transition of graphite domain (sp2 to sp 3 hybridization). These interface- mediated continuous changes in the localized bonding pattern greatly promote the strain-energy dissipation,

leading to a profound tolerance for large strains. Moreover, a size-dependent toughening is demonstrated, attributed to detrimental graphitization and interfacial bond breakage that occur under critically small sp 2 / sp 3 thickness. These findings provide guidance for the experimentally rational design of gradia, and the toughening mechanisms arising from interface-induced electronic structure transition also sheds light on the toughening of other hard but brittle materials through heterophase junctions.

Accession Number: WOS:001340495100003

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Record 159 of 274

Title: Large-scale annotation of biochemically relevant pockets and tunnels in cognate enzyme-ligand complexes

Author(s): Vavra, O (Vavra, O.); Tyzack, J (Tyzack, J.); Haddadi, F (Haddadi, F.); Stourac, J (Stourac, J.); Damborsky, J (Damborsky, J.); Mazurenko, S (Mazurenko, S.); Thornton, JM (Thornton, J. M.); Bednar, D (Bednar, D.)

Source: JOURNAL OF CHEMINFORMATICS **Volume:** 16 **Issue:** 1 **Article Number:** 114 **DOI:** 10.1186/s13321-024-00907-z **Published Date:** 2024 OCT 15

Abstract: Tunnels in enzymes with buried active sites are key structural features allowing the entry of substrates and the release of products, thus contributing to the catalytic efficiency. Targeting the bottlenecks of protein tunnels is also a powerful protein engineering strategy. However, the identification of functional tunnels in multiple protein structures is a non-trivial task that can only be addressed computationally. We present a pipeline integrating automated structural analysis with an in-house machine-learning predictor for the annotation of protein pockets, followed by the calculation of the energetics of ligand transport via biochemically relevant tunnels. A thorough validation using eight distinct molecular systems revealed that CaverDock analysis of ligand un/binding is on par with time-consuming molecular dynamics simulations, but much faster. The optimized and validated pipeline was applied to annotate more than 17,000 cognate enzyme-ligand complexes. Analysis of ligand un/binding energetics indicates that the top priority tunnel has the most favourable energies in 75% of cases. Moreover, energy profiles of cognate ligands revealed that a simple geometry analysis can correctly identify tunnel bottlenecks only in 50% of cases. Our study provides essential information for the interpretation of results from tunnel calculation and energy profiling in mechanistic enzymology and protein engineering. We formulated several simple rules allowing identification of biochemically relevant tunnels based on the binding pockets, tunnel geometry, and ligand transport energy profiles.Scientific contributionsThe pipeline introduced in this work allows for the detailed analysis of a large set of protein-ligand complexes, focusing on transport pathways. We are introducing a novel predictor for determining the relevance of binding pockets for tunnel calculation. For the first time in the field, we present a high-throughput energetic analysis of ligand binding and unbinding, showing that approximate methods for these simulations can identify additional mutagenesis hotspots in enzymes compared to purely geometrical methods. The predictor is included in the supplementary material and can also be accessed at https://github.com/Faranehhad/Large-Scale-Pocket-Tunnel-Annotation.git. The tunnel data calculated in this study has been made publicly available as part of the ChannelsDB 2.0 database, accessible at https://channelsdb2.biodata.ceitec.cz/.

Accession Number: WOS:001332053400001

PubMed ID: 39407342

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ISSN: 1758-2946

Record 160 of 274

Title: From unbound to bound states: Ab initio molecular dynamics of ammonia clusters with an excess electron

Author(s): Turcin, V (Turcin, Vit); Nemirovich, T (Nemirovich, Tatiana); Jungwirth, P (Jungwirth, Pavel)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 161 **Issue:** 14 **Article Number:** 144302 **DOI:** 10.1063/5.0224249 **Published Date:** 2024 OCT 14

Abstract: Ab initio molecular dynamics simulations of negatively charged clusters of 2-48 ammonia molecules were performed to elucidate the electronic stability of the excess electron as a function of cluster size. We show that while the electronic stability of finite temperature clusters increases with cluster size, as few as 5-7 ammonia molecules can bind an excess electron, reaching a vertical binding energy slightly less than half of the bulk value for the largest system studied. These results, which are in agreement with previous studies wherever available, allowed us to analyze the excess electron binding patterns in terms of its radius of gyration and shape anisotropy and provide a qualitative interpretation based on a particle-in-a-spherical-well model.

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PubMed ID: 39378163

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Record 161 of 274

Title: Wide spectral range optical characterization of terbium gallium garnet (TGG) single crystal by universal dispersion model

Author(s): Franta, D (Franta, Daniel); Muresan, MG (Muresan, Mihai-George); Ondracka, P (Ondracka, Pavel); Hroncová, B (Hroncova, Beata); Vizd'a, F (Vizd'a, Frantisek)

Source: OPTICS AND LASER TECHNOLOGY **Volume:** 181 **Article Number:** 111916 **DOI:** 10.1016/j.optlastec.2024.111916 **Early Access Date:** OCT 2024 **Published Date:** 2025 FEB **Part:** C

Abstract: Terbium gallium garnet (TGG - Tb3Ga5O12) 3 Ga 5 O 12) single crystal was optically characterized using the multi-sample and multi-instrument method across a wide spectral range with the help of the universal dispersion model. The obtained optical constants cover the spectral range from the far-IR region (25 cm -1) to the vacuum-UV region (10.3 eV). The applied dispersion model includes all elementary absorption processes occurring within the spectral range that affect the dielectric response, including phonons and valence electron excitations. The primary objective was to accurately determine the optical constants with the highest possible precision. The optical results were compared with ab initio density functional theory calculations to gain insight into the nature of the absorption edge and the distribution of the f-electron excitations.

Accession Number: WOS:001335121600001

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Record 162 of 274

Title: Rugged magneto-hydrodynamic invariants in weakly collisional plasma turbulence: Two-dimensional hybrid simulation results

Author(s): Hellinger, P (Hellinger, Petr); Montagud-Camps, V (Montagud-Camps, Victor)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 690 **Article Number:** A174 **DOI:** 10.1051/0004-6361/202450313 **Published Date:** 2024 OCT 8

Abstract: Aims. We investigated plasma turbulence in the context of solar wind. We concentrated on properties of ideal second-order magneto-hydrodynamic (MHD) and Hall MHD invariants.Methods. We studied the results of a two-dimensional hybrid simulation of decaying plasma turbulence with an initial large cross helicity and a negligible magnetic helicity. We investigated the evolution of the combined energy and the cross, kinetic, mixed, and magnetic helicities. For the combined (kinetic plus magnetic) energy and the cross, kinetic, and mixed helicities, we analysed the corresponding K & aacute;rm & aacute;n-Howarth-Monin (KHM) equation in the hybrid (kinetic proton and fluid electron) approximation.Results. The KHM analysis shows that the combined energy decays at large scales. At intermediate scales, this energy cascades (from large to small scales) via the MHD non-linearity and this cascade partly continues via Hall coupling to sub-ion scales. The cascading combined energy is transferred (dissipated) to the internal energy at small scales via the resistive dissipation and the pressure-strain effect. The Hall term couples the cross helicity with the kinetic one, suggesting that the coupled invariant, referred to here as the mixed helicity, is a relevant turbulence quantity. However, when analysed using the KHM equations, the kinetic and mixed helicities exhibit very dissimilar behaviours to that of the combined energy. On the other hand, the cross helicity, in analogy to the energy, decays at large scales, cascades from large to small scales via the MHD+Hall non-linearity, and is dissipated at small scales via the resistive dissipation and the cross-helicity equivalent of the pressure-strain effect. In contrast to the combined energy, the Hall term is important for the cross helicity over a wide range of scales (even well above ion scales). In contrast, the magnetic helicity is scantily generated through the resistive term and does not exhibit any cascade.

Accession Number: WOS:001331676100029

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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eISSN: 1432-0746

Record 163 of 274

Title: Functionalized composite nanofiber membranes for selective steroid hormone micropollutants uptake from water: Role of cyclodextrin type

Author(s): Imbrogno, A (Imbrogno, Alessandra); Lin, HY (Lin, Han Ya); Gopalakrishnan, A (Gopalakrishnan, Akhil); Minofar, B (Minofar, Babak); Schäfer, AI (Schaefer, Andrea I.)

Source: WATER RESEARCH **Volume:** 267 **Article Number:** 122543 **DOI:** 10.1016/j.watres.2024.122543 **Early Access Date:** OCT 2024 **Published Date:** 2024 DEC 1

Abstract: Cyclodextrins (CD) entrapped in nanofiber composite membranes are potential selective adsorbing materials to remove steroid hormone (SHs) micropollutants from water. This study aims to elucidate the role of CD macrocyclic host type on the SHs inclusion complexation and uptake in

filtration. Three CD types (alpha, (3, and gamma) are crosslinked with epichlorohydrin to form polymers (alpha CDP, (3CDP and gamma CDP) and entrapped into a nanofiber composite membrane by electrospinning. TGA analysis confirmed the CD entrapment into the nanofiber without loss of CD molecules during filtration. The CD type plays a dominant role in controlling the removal of different SHs. A similar removal (range 33 to 50 %) was observed with alpha CDP, irrespective of the SH type. In contrast, removal and uptake dependent on SH type were observed for (3 and gamma CDP, with the highest removal of 74 % for progesterone, followed by estradiol (46 %) and estrone (27 %) and the lowest removal of 3 % for testosterone. Molecular dynamic (MD) simulation revealed a stronger and more stable complex formed with (3CDP, as demonstrated by: i) the closer spatial distribution of SH molecules from the (3CDP cavity and, ii) the quantum chemistry calculations of the lower de-solvation energy (+6.0 kcal/mol), which facilitates the release of water molecules from interacting interface of CD molecule and hormone. Regarding gamma CDP, the highest de-solvation energy (+8.3 kcal/mol) poses an energetic barrier, which hinders the formation of the inclusion complex. In the case of alpha CDP, a higher interaction energy (-8.9 kcal/mol) compared to (3CDP (-4.9 kcal/mol) was obtained, despite the broader spatial distribution observed from the MD simulation attributed to a dominant hydrogen bonding interaction with the OH primary groups on the external surface cavity. The findings highlight the relevance of the CD type in designing selective adsorbing membranes for steroid hormone micropollutant uptake. Experimental results and MD simulation suggest that (3CD is the most suitable CD type for steroid hormone uptake, due to a more stable and stronger inclusion complexation than alpha and gamma CD.

Accession Number: WOS:001332060500001

PubMed ID: 39378729

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ISSN: 0043-1354

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Record 164 of 274

Title: The chromatin remodeler SMARCA5 binds to d-block metal supports: Characterization of affinities by IMAC chromatography and QM analysis

Author(s): Andrikopoulos, PC (Andrikopoulos, Prokopis C.); Cabart, P (Cabart, Pavel)

Source: PLOS ONE **Volume:** 19 **Issue:** 10 **Article Number:** e0309134 **DOI:** 10.1371/journal.pone.0309134 **Published Date:** 2024 OCT 7

Abstract: The ISWI family protein SMARCA5 contains the ATP-binding pocket that coordinates the catalytic Mg2+ ion and water molecules for ATP hydrolysis. In this study, we demonstrate that SMARCA5 can also possess an alternative metal-binding ability. First, we isolated SMARCA5 on the cobalt column (IMAC) to near homogeneity. Examination of the interactions of SMARCA5 with metal-chelating supports showed that, apart from Co2+, it binds to Cu2+, Zn2+ and Ni2+. The efficiency of the binding to the last-listed metal was influenced by the chelating ligand, resulting in a strong preference for Ni-NTA over the Ni-CM-Asp equivalent. To gain insight in the preferential affinity for the Ni-NTA ligand, QM calculations were performed on model systems and metal-ligand complexes with a limited protein fragment of SMARCA5 containing the double-histidine (dHis) motif. The calculations correlated the observed affinity with the relative stability of the d-block metals to tetradentate ligand coordination over tridentate, as well as their overall octahedral coordination capacity. Likewise, binding free energies derived from model imidazole complexes mirrored the observed Ni-NTA/Ni-CM-Asp preferential affinity. Finally, similar calculations on complexes with a SMARCA5 peptide fragment derived from the AlphaFold structural prediction, captured almost accurately the expected relative stability of the TM

complexes, and produced a large energetic separation (similar to 10 kcal center dot mol(-1)) between Ni-NTA and Ni-CM-Asp in favour of the former.

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PubMed ID: 39374200

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ISSN: 1932-6203

Record 165 of 274

Title: Exploring the Role of Excited States' Degeneracy on Vibronic Coupling with Atomic-Scale Optics

Author(s): Vasilev, K (Vasilev, Kirill); Canola, S (Canola, Sofia); Scheurer, F (Scheurer, Fabrice); Boeglin, A (Boeglin, Alex); Lotthammer, F (Lotthammer, Fanny); Chérioux, F (Cherioux, Frederic); Neuman, T (Neuman, Tomas); Schull, G (Schull, Guillaume)

Source: ACS NANO **Volume:** 18 **Issue:** 41 **Pages:** 28052-28059 **DOI:** 10.1021/acsnano.4c07136 **Early Access Date:** OCT 2024 **Published Date:** 2024 OCT 4

Abstract: Interactions between molecular electronic and vibrational states manifest themselves in a variety of forms and have a strong impact on molecular physics and chemistry. For example, the efficiency of energy transfer between organic molecules, ubiquitous in biological systems and in organic optoelectronics, is strongly influenced by vibronic coupling. Using an approach based on scanning tunneling microscope-induced luminescence (STML), we reveal vibronic interactions in optical spectra of a series of single phthalocyanine derivative molecules featuring degenerate or near-degenerate excited states. Based on detailed theoretical simulations, we disentangle spectroscopic signatures belonging to Franck-Condon and Herzberg-Teller vibronic progressions in tip-position-resolved STML spectra, and we directly map out the vibronic coupling between the close-lying excited states of the molecules.

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PubMed ID: 39363581

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Record 166 of 274

Title: Modeling Dipolar Nonprotogenic Solvents with PC-SAFT-Type Equations of State: Pure Substance Properties

Author(s): Klajmon, M (Klajmon, Martin)

Source: JOURNAL OF CHEMICAL AND ENGINEERING DATA **Volume:** 69 **Issue:** 12 **Pages:** 4384-4397 **DOI:** 10.1021/acs.jced.4c00344 **Early Access Date:** OCT 2024 **Published Date:** 2024 OCT 3

Abstract: Dipolar nonprotogenic solvents (DNSs) are interesting and important substances widely used in various applications, including organic syntheses, sustainable fuels, and organic electronics. They exhibit intriguing molecular and interactional properties, characterized by large dipole moments, strong dipole-dipole interactions, hydrogen bond (HB) acceptor ability, and the formation of dimer complexes. The latter aspect, along with the traditional view of DNSs as having a weak or negligible HB donor ability, has led to debates about the origin (dipolar vs HB) of these complexes. Therefore, modeling and predicting the thermodynamic properties of DNSs is challenging and requires sophisticated approaches. The PC-SAFT-type equations of state are powerful tools for describing the macroscopic thermodynamic properties of fluid systems, including DNSs. In this work, we explore and compare the performance of various modeling strategies within PC-SAFT for pure DNSs, including nonpolar, explicitly dipolar, and pseudo-associating approaches. These strategies differ in the treatment of the strongly dipolar character of DNSs. The PC-SAFT parameter sets for each DNS and strategy were determined de novo by fitting them to reliable reference data on the liquid density and vapor pressure. A comprehensive computational evaluation of the results for the fluid-phase thermodynamic properties of six DNSs in their pure form is provided, and the merits and drawbacks of the considered strategies are discussed. The pure-compound parameter values are also analyzed. The best results are obtained from the pseudo-association strategy, which considers DNSs to be self-associating with both HB acceptor and donor sites, followed by an explicitly dipolar approach with optimized dipole moment values. Surprisingly, a nonpolar strategy without any explicit dipolar treatment provides results comparable to those of the above models. It is also demonstrated that optimized or gas-phase dipole moments of DNSs are significantly better for use within PC-SAFT in the context of pure DNSs than those related to the liquid phase calculated quantum-mechanically using a polarizable continuum model. Possible explanations for these observations are provided.

Accession Number: WOS:001328601000001

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ISSN: 0021-9568

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Record 167 of 274

Title: Hybrid TBETI domain decomposition for huge 2D scalar variational inequalities

Author(s): Dostál, Z (Dostal, Zdenek); Sadowská, M (Sadowska, Marie); Horák, D (Horak, David); Kruzík, J (Kruzik, Jakub)

Source: INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN ENGINEERING **Volume:** 125 **Issue:** 24 **DOI:** 10.1002/nme.7597 **Early Access Date:** OCT 2024 **Published Date:** 2024 DEC 30

Abstract: The unpreconditioned H-TFETI-DP (hybrid total finite element tearing and interconnecting dual-primal) domain decomposition method introduced by Klawonn and Rheinbach turned out to be an effective solver for variational inequalities discretized by huge structured grids. The basic idea is to decompose the domain into non-overlapping subdomains, interconnect some adjacent subdomains into clusters on a primal level, and enforce the continuity of the solution across both the subdomain and cluster interfaces by Lagrange multipliers. After eliminating the primal variables, we get a reasonably conditioned quadratic programming (QP) problem with bound and equality constraints. Here, we first reduce the continuous problem to the subdomains' boundaries, then discretize it using the boundary element method, and finally interconnect the subdomains by the averages of adjacent edges. The resulting QP problem in multipliers with a small coarse grid is solved by specialized QP algorithms with optimal complexity. The method can be considered as a three-level multigrid with the coarse grids split between primal and dual variables. Numerical experiments illustrate the efficiency of the presented H-TBETI-DP (hybrid total boundary element tearing and interconnecting dual-primal) method and nice

spectral properties of the discretized Steklov-Poincar & eacute; operators as compared with their finite element counterparts.

Accession Number: WOS:001324133600001

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ISSN: 0029-5981

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Record 168 of 274

Title: Convergence of gut phage communities but not bacterial communities following wild mouse bacteriophage transplantation into captive house mice

Author(s): Cízková, D (Cizkova, Dagmar); Payne, P (Payne, Pavel); Bryjová, A (Bryjova, Anna); Dureje, L (Dureje, Ludovit); Piálek, J (Pialek, Jaroslav); Kreisinger, J (Kreisinger, Jakub)

Source: ISME JOURNAL **Volume:** 18 **Issue:** 1 **Article Number:** wrae178 **DOI:** 10.1093/ismejo/wrae178 **Published Date:** 2024 SEP 30

Abstract: Bacteriophages are abundant components of vertebrate gut microbial communities, impacting bacteriome dynamics, evolution, and directly interacting with the superhost. However, knowledge about gut phageomes and their interaction with bacteriomes in vertebrates under natural conditions is limited to humans and non-human primates. Widely used specific-pathogen-free (SPF) mouse models of host-microbiota interactions have altered gut bacteriomes compared to wild mice, and data on phageomes from wild or other non-SPF mice are lacking. We demonstrate divergent gut phageomes and bacteriomes in wild and captive non-SPF mice, with wild mice phageomes exhibiting higher alpha-diversity and interindividual variability. In both groups, phageome and bacteriome structuring mirrored each other, correlating at the individual level. Re-analysis of previous data from phageomes of SPF mice revealed their enrichment in Suoliviridae crAss-like phages compared to our non-SPF mice. Disrupted bacteriomes in mouse models can be treated by transplanting healthy phageomes, but the effects of phageome transplants on healthy adult gut microbiota are still unknown. We show that experimental transplantation of phageomes from wild to captive mice did not cause major shifts in recipient phageomes. However, the convergence of recipient-to-donor phageomes confirmed that wild phages can integrate into recipient communities. The differences in the subset of integrated phages between the two recipient mouse strains illustrate the context-dependent effects of phage transplantation. The transplantation did not impact recipient gut bacteriomes. This resilience of healthy adult gut microbiomes to the intervention has implications for phage allotransplantation safety.

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PubMed ID: 39276368

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Record 169 of 274

Title: Carboxy-terminal polyglutamylation regulates signaling and phase separation of the Dishevelled protein

Author(s): Kravec, M (Kravec, Marek); Sedo, O (Sedo, Ondrej); Nedvedová, J (Nedvedova, Jana); Micka, M (Micka, Miroslav); Sulcová, M (Sulcova, Marie); Zezula, N (Zezula, Nikodem); Gömöryová, K (Gomoryova, Kristina); Potesil, D (Potesil, David); Ganji, RS (Sri Ganji, Ranjani); Bologna, S (Bologna, Sara); Cervenka, I (Cervenka, Igor); Zdráhal, Z (Zdrahal, Zbynek); Harnos, J (Harnos, Jakub); Tripsianes, K (Tripsianes, Konstantinos); Janke, C (Janke, Carsten); Barinka, C (Barinka, Cyril); Bryja, V (Bryja, Vitezslav)

Source: EMBO JOURNAL **Volume:** 43 **Issue:** 22 **Pages:** 5635-5666 **DOI:** 10.1038/s44318-024-00254-7 **Early Access Date:** SEP 2024 **Published Date:** 2024 NOV 18

Abstract: Polyglutamylation is a reversible posttranslational modification that is catalyzed by enzymes of the tubulin tyrosine ligase-like (TTLL) family. Here, we found that TTLL11 generates a previously unknown type of polyglutamylation that is initiated by the addition of a glutamate residue to the free C-terminal carboxyl group of a substrate protein. TTLL11 efficiently polyglutamylates the Wnt signaling protein Dishevelled 3 (DVL3), thereby changing the interactome of DVL3. Polyglutamylation increases the capacity of DVL3 to get phosphorylated, to undergo phase separation, and to act in the noncanonical Wnt pathway. Both carboxy-terminal polyglutamylation and the resulting reduction in phase separation capacity of DVL3 can be reverted by the deglutamylating enzyme CCP6, demonstrating a causal relationship between TTLL11-mediated polyglutamylation and phase separation. Thus, C-terminal polyglutamylation represents a new type of posttranslational modification, broadening the range of proteins that can be modified by polyglutamylation and providing the first evidence that polyglutamylation can modulate protein phase separation.
Polyglutamylation by the tubulin tyrosine ligase-like (TTLL) family enzymes predominantly regulates cytoskeletal proteins. This study shows that the glutamylase TTLL11 polyglutamylates the Wnt signaling protein Dishevelled 3 (DVL3) at its C-terminus, thus changing its biochemical and signaling properties.TTLL11-mediated polyglutamylation of DVL3 takes place at the alpha-carboxyl group of the terminal methionine and extends the protein with a chain of glutamates.Polyglutamylation of DVL3 regulates its phase separation and phosphorylation.Polyglutamylated DVL3 is more active in the Wnt/planar cell polarity (PCP) pathway.TTLL11 is required for morphogenetic events controlled by PCP in .
Glutamylase TTLL11 catalyzes a novel type of carboxy-terminal polyglutamylation to suppress DVL3 phase separation and enhance its activity in the planar cell polarity pathway.

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PubMed ID: 39349846

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Barinka, Cyril	G-9803-2014	
Tripsianes, Konstantinos	I-8382-2014	
Zezula, Nikodém	KBB-3014-2024	
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Record 170 of 274

Title: Fur microbiome as a putative source of symbiotic bacteria in sucking lice

Author(s): Říhová, JM (Rihova, Jana Martin); Gupta, S (Gupta, Shruti); Nováková, E (Novakova, Eva); Hypsa, V (Hypsa, Vaclav)

Source: SCIENTIFIC REPORTS **Volume:** 14 **Issue:** 1 **Article Number:** 22326 **DOI:** 10.1038/s41598-024-73026-2 **Published Date:** 2024 SEP 27

Abstract: Symbiosis between insects and bacteria has been established countless times. While it is well known that the symbionts originated from a variety of different bacterial taxa, it is usually difficult to determine their environmental source and a route of their acquisition by the host. In this study, we address this question using a model of Neisseriaceae symbionts in rodent lice. These bacteria established their symbiosis independently with different louse taxa (Polyplax, Hoplopleura, Neohaematopinus), most likely from the same environmental source. We first applied amplicon analysis to screen for candidate source bacterium in the louse environment. Since lice are permanent ectoparasites, often specific to the particular host, we screened various microbiomes associated with three rodent species (Microtus arvalis, Clethrionomys glareolus, and Apodemus flavicollis). The analyzed samples included fur, skin, spleen, and other ectoparasites sampled from these rodents. The fur microbiome data revealed a Neisseriaceae bacterium, closely related to the known louse symbionts. The draft genomes of the environmental Neisseriaceae, assembled from all three rodent hosts, converged to a remarkably small size of approximately 1.4 Mbp, being even smaller than the genomes of the related symbionts. Our results suggest that the rodent fur microbiome can serve as a source for independent establishment of bacterial symbiosis in associated louse species. We further propose a hypothetical scenario of the genome evolution during the transition of a free-living bacterium to the member of the rodent fur-associated microbiome and subsequently to the facultative and obligate louse symbionts.

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PubMed ID: 39333204

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Novakova, Eva	D-9475-2016	0000-0003-4090-0655

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Record 171 of 274

Title: BenchStab: a tool for automated querying of web-based stability predictors

Author(s): Velecky, J (Velecky, Jan); Berezny, M (Berezny, Matej); Musil, M (Musil, Milos); Damborsky, J (Damborsky, Jiri); Bednar, D (Bednar, David); Mazurenko, S (Mazurenko, Stanislav)

Source: BIOINFORMATICS **Volume:** 40 **Issue:** 9 **Article Number:** btae553 **DOI:** 10.1093/bioinformatics/btae553 **Published Date:** 2024 SEP 26

Abstract: Protein design requires information about how mutations affect protein stability. Many web-based predictors are available for this purpose, yet comparing them or using them en masse is difficult. Here, we present BenchStab, a console tool/Python package for easy and quick execution of 19 predictors and result collection on a list of mutants. Moreover, the tool is easily extensible with additional predictors. We created an independent dataset derived from the FireProtDB and evaluated 24 different prediction methods.Availability and implementation BenchStab is an open-source Python package available at https://github.com/loschmidt/BenchStab with a detailed README and example usage at https://loschmidt.chemi.muni.cz/benchstab. The BenchStab dataset is available on Zenodo: https://zenodo.org/records/10637728

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Record 172 of 274

Title: What is the true ground state of intermetallic compound Fe₃Al?

Author(s): Vsianská, M (Vsianska, M.); Sob, M (Sob, M.)

Source: SOLID STATE SCIENCES **Volume:** 157 **Article Number:** 107709 **DOI:** 10.1016/j.solidstatesciences.2024.107709 **Early Access Date:** SEP 2024 **Published Date:** 2024 NOV

Abstract: We discuss recent doubts about the true ground-state (GS) structure of the intermetallic compound Fe3Al. It seems that it should be the D0(3) structure (observed experimentally), but there are some considerations that, perhaps, D0(3) might be a high-temperature (>400 K) structure and the GS at 0 K might be the L1(2) structure because there might be a high energy barrier between both structures and, when the temperature is lowered, the system is not able to transform into the (perhaps) lower-energy L1(2) structure. To elucidate this problem, we re-interpret our recent extended ab initio electronic structure calculations for Fe3Al performed with the help of the VASP code and using various exchange-correlation energies within the generalized gradient approximation (GGA). Regrettably, some calculations provide the L1(2) and some of them D0(3) as the GS structure. To resolve this question, we performed further calculations testing 9 frequently applied metaGGAs, such as TPSS, revTPSS, M06-L, SCAN(-L), rSCAN(-L) and r(2)SCAN(-L) representing a higher rung of the Jacob's ladder. It turns out that also here some meta-GGAs lead to L1(2) and some others to D0(3) GS structure and, again, we cannot decide. In this way, the present results represent the very first step on the way to understand the energetics of the Fe3Al compound and its ground state. We hope they may motivate future theoretical and experimental work in this direction.

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Record 173 of 274

Title: Resolving molecular frontier orbitals in molecular junctions with kHz resolution

Author(s): Isshiki, Y (Isshiki, Yuji); Montes, E (Montes, Enrique); Nishino, T (Nishino, Tomoaki); Vazquez, H (Vazquez, Hector); Fujii, S (Fujii, Shintaro)

Source: CHEMICAL SCIENCE **Volume:** 15 **Issue:** 42 **Pages:** 17328-17336 **DOI:** 10.1039/d4sc05285d **Early Access Date:** SEP 2024 **Published Date:** 2024 OCT 30

Abstract: Designing and building single-molecule circuits with tailored functionalities requires a detailed knowledge of the junction electronic structure. The energy of frontier molecular orbitals and their electronic coupling with the electrodes play a key role in determining the conductance of nanoscale molecular circuits. Here, we developed a method for measuring the current-voltage (I-V) characteristics of single-molecule junctions with a time resolution that is two orders of magnitude higher than

previously achieved. These I-V measurements with high temporal resolution, together with atomistic simulations, enabled us to characterize in detail the frontier molecular states and their evolution in sub-angstrom stretching of the junction. For a series of molecules, changes in the electronic structure were resolved as well as their fluctuations prior to junction breakdown. This study describes a new methodology to determine the key frontier MO parameters at single-molecule junctions and demonstrates how these can be mechanically tuned at the single-molecule level.
The current-voltage characteristics of molecular junctions can be measured with a time resolution two orders of magnitude higher than previous methods, allowing detailed characterization of electronic states during mechanical modulation.

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Record 174 of 274

Title: Current perspective towards a general framework to describe and harness friction at the nanoscale

Author(s): Cammarata, A (Cammarata, Antonio); Perviz, E (Perviz, Elliot); Polcar, T (Polcar, Tomas)

Source: PROGRESS IN SURFACE SCIENCE **Volume:** 99 **Issue:** 3 **Article Number:** 100753 **DOI:** 10.1016/j.progsurf.2024.100753 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP

Abstract: Macroscopic friction is the result of the interplay of several processes occurring at different scales; an atom-scale description of the tribological interactions is then paramount for the explanation of the elementary phenomena at the basis of such processes, and finds immediate application in technological fields involving nanostructured devices. At the moment, there is no theory which tells us what is the friction coefficient given the atomic description of two surfaces in contact: it is measured experimentally or computationally case by case at specific environmental parameters and chemical composition of the moving surfaces. A general theory describing nanoscale friction is then desirable to reduce human effort, search time and material costs necessary to design new tribological materials with target response. We here provide a selective overview of theoretical and computational models which, from our perspective, may pave the avenue towards a unified theoretical framework of nanofriction. In this respect, we believe that the key aspect is to identify a novel mathematical formulation of friction based on its energetic aspects, i.e. energy dissipation, rather than its dynamical effects, i.e. hindering the relative motion of interacting surfaces. Ultimately, such avenue might lead to a way to predict the value of the friction coefficient of two surfaces in contact from the sole knowledge of the atom types and their arrangement, without the need to measure it in operative conditions: one of the biggest challenges in the field of nanotribology.

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Record 175 of 274

Title: Harnessing Ti₃C₂-WS₂ nanostructures as efficient energy scaffoldings for photocatalytic hydrogen generation

Author(s): Subramani, A (Subramani, Amutha); Chacko, L (Chacko, Levna); Wu, B (Wu, Bing); Mazánek, V (Mazanek, Vlastimil); Senthil, C (Senthil, Chenrayan); Mourdikoudis, S (Mourdikoudis, Stefanos); Sofer, Z (Sofer, Zdenek)

Source: MATERIALS TODAY SUSTAINABILITY **Volume:** 28 **Article Number:** e100964 **DOI:** 10.1016/j.mtsust.2024.100964 **Early Access Date:** SEP 2024 **Published Date:** 2024 DEC

Abstract: Two-dimensional (2D) Ti3C2 MXene have attracted a lot of attention as frontier materials for the development of effective photocatalysts that can transform solar energy into chemical energy, which is essential for water splitting to produce hydrogen. Here, we use first principle calculations to understand the structural, electronic, and vibrational features of a novel heterostructure comprising a monolayer of tungsten disulfide (WS2) and titanium carbide (Ti3C2) MXene. Our theoretical calculations revealed that the Ti3C2 maximizes the interfacial contact area with the WS2 monolayer creating a strong p-d hybridization for the WS2/Ti3C2 heterostructure. As a result, a well-constructed Schottky junction is enabled, facilitating an interconnected electron pathway across the interface which is conducive for an efficient photocatalytic performance. Further, the experimentally designed WS2/Ti3C2 heterostructure and its photocatalytic activity based on the synergistic action between MXene and WS2 is investigated. Optical properties calculated are compared with experimental data derived from UV-Visible spectroscopy. The excellent conductivity and stability along with the light absorption in the visible region of WS2/Ti3C2 enhances the photocatalytic performance approaching photocurrent densities of similar to 33 and 120 mu A/cm(2) in the HER and OER region, respectively. Overall, the present research not only improves our understanding of WS2/Ti3C2 heterostructure for an improved photocatalytic activity, but also provides an efficient method toward sustainable hydrogen production.

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Record 176 of 274

Title: The explicit bonding reaction ensemble Monte Carlo method

Author(s): Blanco, PM (Blanco, Pablo M.); Kosovan, P (Kosovan, Peter)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 161 **Issue:** 9 **Article Number:** 094906 **DOI:** 10.1063/5.0226122 **Published Date:** 2024 SEP 7

Abstract: We present the explicit bonding Reaction ensemble Monte Carlo (eb-RxMC) method, designed to sample reversible bonding reactions in macromolecular systems in thermodynamic equilibrium. Our eb-RxMC method is based on the reaction ensemble method; however, its implementation differs from the latter by the representation of the reaction. In the eb-RxMC implementation, we are adding or deleting bonds between existing particles, instead of inserting or deleting particles with different chemical identities. This new implementation makes the eb-RxMC method suitable for simulating the formation of reversible linkages between macromolecules, which

would not be feasible with the original implementation. To enable coupling of our eb-RxMC algorithm with molecular dynamics algorithm for the sampling of the configuration space, we biased the sampling of reactions only within a certain inclusion radius. We validated our algorithm using a set of ideally behaving systems undergoing dimerization and polycondensation reactions, for which analytical results are available. For dimerization reactions with various equilibrium constants and initial compositions, the degree of conversion measured in our simulations perfectly matched the reference values given by the analytical equations. We also showed that this agreement is not affected by the arbitrary choice of the inclusion radius or the stiffness of the harmonic bond potential. Next, we showed that our simulations can correctly match the analytical results for the distribution of the degree of polymerization and end-to-end distance of ideal chains in polycondensation reactions. Altogether, we demonstrated that our eb-RxMC simulations correctly sample both reaction and configuration spaces of these reference systems, opening the door to future simulations of more complex interacting macromolecular systems.

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PubMed ID: 39225533

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Record 177 of 274

Title: Sessile ⟨100⟩ self-interstitial clusters with non-parallel edge dumbbells in irradiated bcc Fe and other metals

Author(s): Klaver, TPC (Klaver, T. P. C.); Domain, C (Domain, C.); Becquart, CS (Becquart, C. S.)

Source: SCRIPTA MATERIALIA **Volume:** 255 **Article Number:** 116353 **DOI:** 10.1016/j.scriptamat.2024.116353 **Early Access Date:** SEP 2024 **Published Date:** 2025 JAN 15

Abstract: Density Functional Theory calculations of self-interstitial atom clusters in bcc Fe unexpectedly show that from similar to 9-14 self-interstitial atoms, an intriguing new family of sessile < 100 > clusters, surrounded by < 110 > dumbbells, are more stable than highly mobile clusters of parallel < 111 > dumbbells. The < 110 > edge dumbbells find a favorable location in terms of strain energy on the tensile side around the edges of the < 100 > center, thus stabilizing the clusters. These sessile clusters might explain resistivity recovery results that suggested an absence of glissile self-interstitial clusters up to large cluster sizes in irradiated Fe, while smaller self-interstitial atom clusters likely would have been present. The mechanism of non-parallel edge interstitials stabilizing an otherwise higher energy interstitial loop is also found in some fcc metals.

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Record 178 of 274

Title: Loss of ADAR1 protein induces changes in small RNA landscape in hepatocytes

Author(s): Roucová, K (Roucova, Kristina); Vopálensky, V (Vopalensky, Vaclav); Masek, T (Masek, Tomas); Del Llano, E (Del Llano, Edgar); Provazník, J (Provaznik, Jan); Landry, JJM (Landry, Jonathan J. M.); Azevedo, N (Azevedo, Nayara); Ehler, E (Ehler, Edvard); Benes, V (Benes, Vladimir); Pospísek, M (Pospisek, Martin)

Source: RNA **Volume:** 30 **Issue:** 9 **Pages:** 1164-1183 **DOI:** 10.1261/rna.080097.124 **Published Date:** 2024 SEP

Abstract: In recent years, numerous evidence has been accumulated about the extent of A-to-I editing in human RNAs and the key role ADAR1 plays in the cellular editing machinery. It has been shown that A-to-I editing occurrence and frequency are tissue-specific and essential for some tissue development, such as the liver. To study the effect of ADAR1 function in hepatocytes, we have created Huh7.5 ADAR1 KO cell lines. Upon IFN treatment, the Huh7.5 ADAR1 KO cells show rapid arrest of growth and translation, from which they do not recover. We analyzed translatome changes by using a method based on sequencing of separate polysome profile RNA fractions. We found significant changes in the transcriptome and translatome of the Huh7.5 ADAR1 KO cells. The most prominent changes include negatively affected transcription by RNA polymerase III and the deregulation of snoRNA and Y RNA levels. Furthermore, we observed that ADAR1 KO polysomes are enriched in mRNAs coding for proteins pivotal in a wide range of biological processes such as RNA localization and RNA processing, whereas the unbound fraction is enriched mainly in mRNAs coding for ribosomal proteins and translational factors. This indicates that ADAR1 plays a more relevant role in small RNA metabolism and ribosome biogenesis.

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Record 179 of 274

Title: Integrating Newton's equations of motion in the reciprocal space

Author(s): Cammarata, A (Cammarata, Antonio); Dasic, M (Dasic, Miljan); Nicolini, P (Nicolini, Paolo)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 161 **Issue:** 8 **Article Number:** 084111 **DOI:** 10.1063/5.0224108 **Published Date:** 2024 AUG 28

Abstract: We here present the normal dynamics technique, which recasts the Newton's equations of motion in terms of phonon normal modes by exploiting a proper sampling of the reciprocal space. After introducing the theoretical background, we discuss how the reciprocal space sampling enables us to (i) obtain a computational speedup by selecting which and how many wave vectors of the Brillouin zone will be considered and (ii) account for distortions realized across large atomic distances without the use of large simulation cells. We implemented the approach into an open-source code, which we used to present three case studies: in the first one, we elucidate the general strategy for the sampling of the reciprocal space; in the second one, we illustrate the potential of the approach by studying the stabilization effect of temperature in alpha-uranium; and in the last one, we investigate the characterization of Raman spectra at different temperatures in MoS2/MX2 transition metal dichalcogenide heterostructures. Finally, we discuss how the procedure is general and can be used to simulate periodic, semiperiodic, and finite systems such as crystals, slabs, nanoclusters, or molecules.

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Record 180 of 274

Title: Fixed point results in intuitionistic fuzzy pentagonal controlled metric spaces with applications to dynamic market equilibrium and satellite web coupling

Author(s): Ishtiaq, U (Ishtiaq, Umar); Alshaikey, S (Alshaikey, Salha); Riaz, MB (Riaz, Muhammad Bilal); Ahmad, K (Ahmad, Khaleel)

Source: PLOS ONE **Volume:** 19 **Issue:** 8 **Article Number:** e0303141 **DOI:** 10.1371/journal.pone.0303141 **Published Date:** 2024 AUG 28

Abstract: This manuscript contains several new spaces as the generalizations of fuzzy triple controlled metric space, fuzzy controlled hexagonal metric space, fuzzy pentagonal controlled metric space and intuitionistic fuzzy double controlled metric space. We prove the Banach fixed point theorem in the context of intuitionistic fuzzy pentagonal controlled metric space, which generalizes the previous ones in the existing literature. Further, we provide several non-trivial examples to support the main results. The capacity of intuitionistic fuzzy pentagonal controlled metric spaces to model hesitation, capture dual information, handle imperfect information, and provide a more nuanced representation of uncertainty makes them important in dynamic market equilibrium. In the context of changing market dynamics, these aspects contribute to a more realistic and flexible modelling approach. We present an application to dynamic market equilibrium and solve a boundary value problem for a satellite web coupling.

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Record 181 of 274

Title: Unraveling the Interface Chemistry between HCN and Cosmic Silicates by the Interplay of Infrared Spectroscopy and Quantum Chemical Modeling

Author(s): Bancone, N (Bancone, Niccolo); Santalucia, R (Santalucia, Rosangela); Pantaleone, S (Pantaleone, Stefano); Ugliengo, P (Ugliengo, Piero); Mino, L (Mino, Lorenzo); Rimola, A (Rimola, Albert); Corno, M (Corno, Marta)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 128 **Issue:** 36 **Pages:** 15171-15178 **DOI:** 10.1021/acs.jpcc.4c03454 **Early Access Date:** AUG 2024 **Published Date:** 2024 AUG 20

Abstract: Understanding the interaction between hydrogen cyanide (HCN) and silicate surfaces is crucial for elucidating the prebiotic processes occurring on interstellar grain cores as well as in cometary and meteoritic matrices. In this study, we characterized the adsorption features of HCN on crystalline forsterite (Mg_2SiO_4) surfaces, one of the most abundant cosmic silicates, by combining experimental

infrared spectra at low temperatures (100-150 K) with periodic DFT simulations. Results showed the coexistence of both molecular and dissociative HCN adsorption complexes as a function of the considered forsterite crystalline face. Molecular adsorptions dominate on the most stable surfaces, while dissociative adsorptions occur predominantly on surfaces of lower stability, catalyzed by the enhanced Lewis acid-base behavior of surface-exposed Mg2+-O2- ion pairs. On the whole set of adsorption cases, harmonic frequency calculations were carried out and compared with the experimental infrared bands. To disentangle each vibrational mode contributing to the experimental broad bands, we run the best nonlinear fit between the predicted set of frequencies and the experimental bands. The outcome of this procedure allowed us to (i) deconvolute the experimental IR spectrum by assigning computed normal modes of vibrations to the main features of each band and (ii) reveal which crystal faces are responsible for the largest contribution to the adsorbate vibrational bands, giving information about the morphology of the samples. The present straightforward procedure is quite general and of broad interest in the fine characterization of the infrared spectra of adsorbates on complex inorganic material surfaces.

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Record 182 of 274

Title: Investigation of mesoscopic boundary conditions for lattice Boltzmann method in laminar flow problems

Author(s): Eichler, P (Eichler, Pavel); Fucik, R (Fucik, Radek); Strachota, P (Strachota, Pavel)

Source: COMPUTERS & MATHEMATICS WITH APPLICATIONS **Volume:** 173 **Pages:** 87-101 **DOI:** 10.1016/j.camwa.2024.08.009 **Early Access Date:** AUG 2024 **Published Date:** 2024 NOV 1

Abstract: For use with the lattice Boltzmann method, the macroscopic boundary conditions need to be transformed into their mesoscopic counterparts. Commonly used mesoscopic boundary conditions use the equilibrium density function, which introduces undesirable artifacts into the numerical solution, especially near interfaces with other types of boundary conditions. In this work, several variants of the mesoscopic boundary conditions are summarized and numerically investigated by means of benchmark problems for the incompressible Navier-Stokes equations with known analytical solutions. To improve the numerical approximation of the velocity and pressure fields, moment-based boundary conditions are extended for the D3Q27 velocity model. Furthermore, the interpolated boundary conditions are improved. These newly developed boundary conditions are shown to produce results with a substantially smaller numerical error.

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Record 183 of 274

Title: The hare syphilis agent is related to, but distinct from, the treponeme causing rabbit syphilis

Author(s): Pospísilová, P (Pospisilova, Petra); Cejková, D (Cejkova, Darina); Bursíková, P (Bursikova, Pavla); Fedrová, P (Fedrova, Pavla); Mikalová, L (Mikalova, Lenka); Najt, D (Najt, David); Tom, N (Tom, Nikola); Hisgen, L (Hisgen, Linda); Lueert, S (Lueert, Simone); Lumeij, JT (Lumeij, Johannes T.); Ågren, EO (Agren, Erik O.); Knauf, S (Knauf, Sascha); Smajs, D (Smajs, David)

Source: PLOS ONE **Volume:** 19 **Issue:** 8 **Article Number:** e0307196 **DOI:** 10.1371/journal.pone.0307196 **Published Date:** 2024 AUG 12

Abstract: The treponemes infecting lagomorphs include Treponema paraluisleporidarum ecovar Cuniculus (TPeC) and ecovar Lepus (TPeL), infecting rabbits and hares, respectively. In this study, we described the first complete genome sequence of TPeL, isolate V3603-13, from an infected mountain hare (Lepus timidus) in Sweden. In addition, we determined 99.0% of the genome sequence of isolate V246-08 (also from an infected mountain hare, Sweden) and 31.7% of the genome sequence of isolate Z27 A77/78 (from a European hare, Lepus europeaus, The Netherlands). The TPeL V3603-13 genome had considerable gene synteny with the TPeC Cuniculi A genome and with the human pathogen T. pallidum, which causes syphilis (ssp. pallidum, TPA), yaws (ssp. pertenue, TPE) and endemic syphilis (ssp. endemicum, TEN). Compared to the TPeC Cuniculi A genome, TPeL V3603-13 contained four insertions and 11 deletions longer than three nucleotides (ranging between 6 and2,932 nts). In addition, there were 25 additional indels, from one to three nucleotides long, altogether spanning 36 nts. The number of single nucleotide variants (SNVs) between TPeC Cuniculi A and TPeL V3603-13 were represented by 309 nucleotide differences. Major proteome coding differences between TPeL and TPeC were found in the tpr gene family, and (predicted) genes coding for outer membrane proteins, suggesting that these components are essential for host adaptation in lagomorph syphilis. The phylogeny revealed that the TPeL sample from the European brown hare was more distantly related to TPeC Cuniculi A than V3603-13 and V246-08.

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Record 184 of 274

Title: Tapinarof and its structure-activity relationship for redox chemistry and phototoxicity on human skin keratinocytes

Author(s): Zatloukalova, M (Zatloukalova, Martina); Hanyk, J (Hanyk, Jiri); Papouskova, B (Papouskova, Barbora); Kabelac, M (Kabelac, Martin); Vostalova, J (Vostalova, Jitka); Vacek, J (Vacek, Jan)

Source: FREE RADICAL BIOLOGY AND MEDICINE **Volume:** 223 **Pages:** 212-223 **DOI:** 10.1016/j.freeradbiomed.2024.07.032 **Early Access Date:** AUG 2024 **Published Date:** 2024 OCT

Abstract: Tapinarof (3,5-dihydroxy-4-isopropylstilbene) is a therapeutic agent used in the treatment of psoriasis (VTAMA (R)). In this study, we examined the redox behaviour, (photo)stability, (photo)toxicity and (bio)transformation of tapinarof in the context of a structure-activity relationship study. Selected derivatives of the structurally related tapinarof were investigated, namely resveratrol, pterostilbene, pinosylvin and its methyl ether. Tapinarof undergoes electrochemical oxidation in a neutral aqueous medium at a potential of around +0.5 V (vs. Ag|AgCl|3M KCl). The anodic reaction of this substance is a proton-dependent irreversible and adsorption-driven process. The pKa value of tapinarof corresponds to 9.19 or 9.93, based on empirical and QM calculation approach, respectively. The oxidation potentials of tapinarof and its analogues correlate well with their HOMO (highest occupied molecular orbital) energy level. The ability to scavenge the DPPH radical decreased in the order trolox >= resveratrol > pterostilbene > tapinarof > pinosylvin >> pinosylvin methyl ether. It was also confirmed that tapinarof, being a moderate electron donor, is able to scavenge the ABTS radical and inhibit lipid peroxidation. The 4 '-OH group plays a pivotal role in antioxidant action of stilbenols. During the stability studies, it was shown that tapinarof is subject to spontaneous degradation under aqueous conditions, and its degradation is accelerated at elevated temperatures and after exposure to UVA (315-399 nm) radiation. In aqueous media at pH 7.4, we observed an similar to 50 % degradation of tapinarof after 48 h at laboratory temperature. The main UVA photodegradation processes include dihydroxylation and hydration. In conclusion, the phototoxic effect of tapinarof on a human keratinocytes cell line (HaCaT) was evaluated. Tapinarof exhibited a clear phototoxic effect, similar to phototoxic standard chlorpromazine. The IC50 values of the cytotoxicity and phototoxic effects of tapinarof correspond to 27.6 and 3.7 mu M, respectively. The main HaCaT biotransformation products of tapinarof are sulfates and glucuronides.

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Record 185 of 274

Title: Computational Design of Pore-Forming Peptides with Potent Antimicrobial and Anticancer Activities

Author(s): Deb, R (Deb, Rahul); Torres, MDT (Torres, Marcelo D. T.); Boudny, M (Boudny, Miroslav); Koberská, M (Koberska, Marketa); Cappiello, F (Cappiello, Floriana); Popper, M (Popper, Miroslav); Bendová, KD (Bendova, Katerina Dvorakova); Drabinová, M (Drabinova, Martina); Hanácková, A (Hanackova, Adelheid); Jeannot, K (Jeannot, Katy); Petrík, M (Petrik, Milos); Mangoni, ML (Mangoni, Maria Luisa); Novotná, GB (Novotna, Gabriela Balikova); Mráz, M (Mraz, Marek); de la Fuente-nunez, C (de la Fuente-nunez, Cesar); Vácha, R (Vacha, Robert)

Source: JOURNAL OF MEDICINAL CHEMISTRY **Volume:** 67 **Issue:** 16 **Pages:** 14040-14061 **DOI:** 10.1021/acs.jmedchem.4c00912 **Early Access Date:** AUG 2024 **Published Date:** 2024 AUG 8

Abstract: Peptides that form transmembrane barrel-stave pores are potential alternative therapeutics for bacterial infections and cancer. However, their optimization for clinical translation is hampered by a lack of sequence-function understanding. Recently, we have de novo designed the first synthetic barrel-stave pore-forming antimicrobial peptide with an identified function of all residues. Here, we systematically mutate the peptide to improve pore-forming ability in anticipation of enhanced activity. Using computer simulations, supported by liposome leakage and atomic force microscopy experiments, we find that pore-forming ability, while critical, is not the limiting factor for improving activity in the submicromolar range. Affinity for bacterial and cancer cell membranes needs to be optimized simultaneously. Optimized peptides more effectively killed antibiotic-resistant ESKAPEE bacteria at submicromolar concentrations, showing low cytotoxicity to human cells and skin model. Peptides showed systemic anti-infective activity in a preclinical mouse model of Acinetobacter baumannii infection. We also demonstrate peptide optimization for pH-dependent antimicrobial and anticancer activity.

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Record 186 of 274

Title: Electrochemical stability of biodegradable Zn-Cu alloys through machine-learning accelerated high-throughput discovery

Author(s): Luo, K (Luo, Kun); Liu, ZR (Liu, Zhaorui); Yu, R (Yu, Rui); Xu, TF (Xu, Tengfei); Legut, D (Legut, Dominik); Yin, X (Yin, Xing); Zhang, RF (Zhang, Ruifeng)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 26 **Issue:** 35 **Pages:** 23010-23022 **DOI:** 10.1039/d4cp02307b **Early Access Date:** AUG 2024 **Published Date:** 2024 SEP 11

Abstract: Zn-Cu alloys have attracted great attention as biodegradable alloys owing to their excellent mechanical properties and biocompatibility, with corrosion characteristics being crucial for their suitability for biomedical applications. However, the unresolved identification of intermetallic compounds in Zn-Cu alloys affecting corrosion and the complexity of the application environment hamper the understanding of their electrochemical behavior. Utilizing high-throughput first-principles calculations and machine-learning accelerated evolutionary algorithms for screening the most stable compounds in Zn-Cu systems, a dataset encompassing the formation energy of 2033 compounds is generated. It reveals that most of the experimentally reported Zn-Cu compounds can be replicated, especially the structure of R32 CuZn5 is first discovered which possesses the lowest formation energy of -0.050 eV per atom. Furthermore, the simulated X-ray diffraction pattern matches perfectly with the experimental ones. By formulating 342 potential electrochemical reactions based on the binary compounds, the Pourbaix diagrams for Zn-Cu alloys are constructed to clarify the fundamental competition between different phases and ions. The calculated equilibrium potential of CuZn5 is higher than that of Zn through the forward reaction Zn + CuZn5 reversible arrow CuZn5 + Zn2+ + 2e(-), resulting in microcell formation owing to the stronger charge density localization in Zn compared to CuZn5. The presence of chlorine accelerates the corrosion of Zn through the reaction Zn + CuZn5 + 6Cl(-) + 6H(2)O reversible arrow Cu + 6ZnOHCl + 6H(+) + 12e(-), where the formation of ZnOHCl disrupts the ZnO passive film and expands the corrosion pH range from 9.2 to 8.8. Our findings reveal an accurate quantitative corrosion mechanism for Zn-Cu alloys, providing an effective pathway to investigate the corrosion resistance of biodegradable alloys.

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Record 187 of 274

Title: Tubulin Vibration Modes Are in the Subterahertz Range, and Their Electromagnetic Absorption Is Affected by Water

Author(s): Pandey, SK (Pandey, Saurabh Kumar); Cifra, M (Cifra, Michal)

Source: JOURNAL OF PHYSICAL CHEMISTRY LETTERS **Volume:** 15 **Issue:** 32 **Pages:** 8334-8342 **DOI:** 10.1021/acs.jpclett.4c01553 **Early Access Date:** AUG 2024 **Published Date:** 2024 AUG 7

Abstract: Many proteins are thought to coordinate distant sites in their structures through a concerted action of global structural vibrations. However, the direct experimental spectroscopic detection of these vibration modes is rather elusive. We used normal-mode analysis to explore the dominant vibration modes of an all-atom model of the tubulin protein and described their characteristics using a large ensemble of tubulin structures. We quantified the frequency range of the normal vibrational modes to be in the subterahertz band, specifically between similar to 40 and similar to 160 GHz. Adding water layers to the model increases the frequencies of the low-frequency modes and narrows the frequency variations of the modes among the protein ensemble. We also showed how the electromagnetic absorption of tubulin vibration modes is affected by vibrational damping. These results contribute to our understanding of tubulin's vibrational and electromagnetic properties and provide a foundation for future attempts to control protein behavior via external electromagnetic fields.

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ISSN: 1948-7185

Record 188 of 274

Title: Tissue-specific sex-dependent difference in the metabolism of fatty acid esters of hydroxy fatty acids

Author(s): Riecan, M (Riecan, Martin); Domanska, V (Domanska, Veronika); Lupu, C (Lupu, Cristina); Patel, M (Patel, Maulin); Vondrackova, M (Vondrackova, Michaela); Rossmeisl, M (Rossmeisl, Martin); Saghatelian, A (Saghatelian, Alan); Lupu, F (Lupu, Florea); Kuda, O (Kuda, Ondrej)

Source: BIOCHIMICA ET BIOPHYSICA ACTA-MOLECULAR AND CELL BIOLOGY OF LIPIDS **Volume:** 1869 **Issue:** 8 **Article Number:** 159543 **DOI:** 10.1016/j.bbalip.2024.159543 **Early Access Date:** AUG 2024 **Published Date:** 2024 DEC

Abstract: Fatty acid esters of hydroxy fatty acids (FAHFAs) are endogenous bioactive lipids known for their antiinflammatory and anti-diabetic properties. Despite their therapeutic potential, little is known about the sexspecific variations in FAHFA metabolism. This study investigated the role of sex and Androgen Dependent TFPI Regulating Protein (ADTRP), a FAHFA hydrolase. Additionally, tissue-specific differences in FAHFA levels, focusing on the perigonadal white adipose tissue (pgWAT), subcutaneous white adipose tissue (scWAT), brown adipose tissue (BAT), plasma, and liver, were evaluated using metabolomics and lipidomics. We found that female mice exhibited higher FAHFA

levels in pgWAT, scWAT, and BAT compared to males. FAHFA levels were inversely related to testosterone and Adtrp mRNA, which showed significantly lower expression in females compared with males in pgWAT and scWAT. However, no significant differences between the sexes were observed in plasma and liver FAHFA levels. Adtrp deletion had minimal impact on both sexes' metabolome and lipidome of pgWAT. However, we discovered higher endogenous levels of triacylglycerol estolides containing FAHFAs, a FAHFA metabolic reservoir, in the pgWAT of female mice. These findings suggest that sex-dependent differences in FAHFA levels occur primarily in specific WAT depots and may modulate local insulin sensitivity in adipocytes, and the role of ADTRP is limited to adipose depots. However, further investigations are warranted to fully comprehend the underlying mechanisms and implications of sex-dependent regulation of human FAHFA metabolism.

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PubMed ID: 39097081

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Record 189 of 274

Title: A consequential one-night stand: Episodic historical hybridization leads to mitochondrial takeover in sympatric desert ant-eating spiders

Author(s): Ortiz, D (Ortiz, David); Pekár, S (Pekar, Stano); Dianat, M (Dianat, Malahat)

Source: MOLECULAR PHYLOGENETICS AND EVOLUTION **Volume:** 199 **Article Number:** 108167 **DOI:** 10.1016/j.ympev.2024.108167 **Early Access Date:** AUG 2024 **Published Date:** 2024 OCT

Abstract: Disentangling the genomic intricacies underlying speciation and the causes of discordance between sources of evidence can offer remarkable insights into evolutionary dynamics. The ant-eating spider Zodarion nitidum, found across the Middle East and Egypt, displays yellowish and blackish morphs that co-occur sympatrically. These morphs additionally differ in behavioral and physiological features and show complete pre-mating reproductive isolation. In contrast, they possess similar sexual features and lack distinct differences in their mitochondrial DNA. We analyzed both Z. nitidum morphs and outgroups using genome-wide and additional mitochondrial DNA data. The genomic evidence indicated that Yellow and Black are reciprocally independent lineages without signs of recent admixture. Interestingly, the sister group of Yellow is not Black but Z. luctuosum, a morphologically distinct species. Genomic gene flow analyses pinpointed an asymmetric nuclear introgression event, with Yellow contributing nearly 5 % of its genome to Black roughly 320,000 years ago, intriguingly aligning with the independently estimated origin of the mitochondrial DNA of Black. We conclude that the blackish and yellowish morphs of Z. nitidum are long-diverged distinct species, and that the ancient and modest genomic introgression event registered resulted in a complete mitochondrial takeover of Black by Yellow. This investigation underscores the profound long-term effects that even modest hybridization events can have on the genome of organisms. It also exemplifies the utility of phylogenetic networks for estimating historical events and how integrating independent lines of evidence can increase the reliability of such estimations.

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Record 190 of 274

Title: Real Time Tracking of Nanoconfined Water-Assisted Ion Transfer in Functionalized Graphene Derivatives Supercapacitor Electrodes

Author(s): Padinjareveetil, AKK (Padinjareveetil, Akshay Kumar K.); Pykal, M (Pykal, Martin); Bakandritsos, A (Bakandritsos, Aristides); Zboril, R (Zboril, Radek); Otyepka, M (Otyepka, Michal); Pumera, M (Pumera, Martin)

Source: ADVANCED SCIENCE **Volume:** 11 **Issue:** 39 **DOI:** 10.1002/advs.202307583 **Early Access Date:** AUG 2024 **Published Date:** 2024 OCT

Abstract: Water molecules confined in nanoscale spaces of 2D graphene layers have fascinated researchers worldwide for the past several years, especially in the context of energy storage applications. The water molecules exchanged along with ions during the electrochemical process can aid in wetting and stabilizing the layered materials resulting in an anomalous enhancement in the performance of supercapacitor electrodes. Engineering of 2D carbon electrode materials with various functionalities (oxygen (& horbar;O), fluorine (& horbar;F), nitrile (& horbar;C equivalent to N), carboxylic (& horbar;COOH), carbonyl (& horbar;C & boxH;O), nitrogen (& horbar;N)) can alter the ion/water organization in graphene derivatives, and eventually their inherent ion storage ability. Thus, in the current study, a comparative set of functionalized graphene derivatives-fluorine-doped cyanographene (G-F-CN), cyanographene (G-CN), graphene acid (G-COOH), oxidized graphene acid (G-COOH (O)) and nitrogen superdoped graphene (G-N) is systematically evaluated toward charge storage in various aqueous-based electrolyte systems. Differences in functionalization on graphene derivatives influence the electrochemical properties, and the real-time mass exchange during the electrochemical process is monitored by electrochemical quartz crystal microbalance (EQCM). Electrogravimetric assessment revealed that oxidized 2D acid derivatives (G-COOH (O)) are shown to exhibit high ion storage performance along with maximum water transfer during the electrochemical process. The complex understanding of the processes gained during supercapacitor electrode charging in aqueous electrolytes paves the way toward the rational utilization of graphene derivatives in forefront energy storage applications.
Covalent functionalization and doping of graphene surfaces -featuring groups such as oxygen, cyano-, carbon-fluorine, carboxyl groups, and nitrogen heteroatoms- significantly affects water-assisted ion transfer as monitored with electrochemical quartz crystal microbalance, modulating the performance of supercapacitor electrodes. Such studies are crucial for advancing energy storage applications with a broader impact across electrochemistry-related technological domains. image

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Record 191 of 274

Title: Impact of intrapartum antibiotic prophylaxis on the oral and fecal bacteriomes of children in the first week of life

Author(s): Pivrncova, E (Pivrncova, Eliska); Buresova, L (Buresova, Lucie); Kotaskova, I (Kotaskova, Iva); Videnska, P (Videnska, Petra); Andryskova, L (Andryskova, Lenka); Piler, P (Piler, Pavel); Janku, P (Janku, Petr); Borek, I (Borek, Ivo); Bohm, J (Bohm, Jan); Klanova, J (Klanova, Jana); Budinska, E (Budinska, Eva); Linhartova, P (Linhartova, Petra Borilova)

Source: SCIENTIFIC REPORTS **Volume:** 14 **Issue:** 1 **Article Number:** 18163 **DOI:** 10.1038/s41598-024-68953-z **Published Date:** 2024 AUG 6

Abstract: Intrapartum antibiotic prophylaxis (IAP) is commonly used during C-section delivery and in Group B Streptococcus-positive women before vaginal delivery. Here, we primarily aimed to investigate the effect of IAP on the neonatal oral and fecal bacteriomes in the first week of life. In this preliminary study, maternal and neonatal oral swabs and neonatal fecal (meconium and transitional stool) swabs were selected from a pool of samples from healthy mother-neonate pairs participating in the pilot phase of CELSPAC: TNG during their hospital stay. The DNA was extracted and bacteriome profiles were determined by 16S rRNA amplicon sequencing (Illumina). In the final dataset, 33 mother-neonate pairs were exposed to antibiotics during C-section or vaginal delivery (cases; +IAP) and the vaginal delivery without IAP (controls, -IAP) took place in 33 mother-neonate pairs. Differences in alpha diversity (Shannon index, $p=0.01$) and bacterial composition (PERMANOVA, $p<0.05$) between the +IAP and -IAP groups were detected only in neonatal oral samples collected <= 48 h after birth. No significant differences between meconium bacteriomes of the +IAP and -IAP groups were observed ($p>0.05$). However, the IAP was associated with decreased alpha diversity (number of amplicon sequence variants, $p<0.001$), decreased relative abundances of the genera Bacteroides and Bifidobacterium, and increased relative abundances of genera Enterococcus and Rothia ($q<0.01$ for all of them) in transitional stool samples. The findings of this study suggest that exposure to IAP may significantly influence the early development of the neonatal oral and gut microbiomes. IAP affected the neonatal oral bacteriome in the first two days after birth as well as the neonatal fecal bacteriome in transitional stool samples. In addition, it highlights the necessity for further investigation into the potential long-term health impacts on children.

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Record 192 of 274

Title: Streamlining NMR Chemical Shift Predictions for Intrinsically Disordered Proteins: Design of Ensembles with Dimensionality Reduction and Clustering

Author(s): Bakker, MJ (Bakker, Michael J.); Gaffour, A (Gaffour, Amina); Juhás, M (Juhas, Martin); Zapletal, V (Zapletal, Vojtech); Stosek, J (Stosek, Jakub); Bratholm, LA (Bratholm, Lars A.); Precechtelova, JP (Precechtelova, Jana Pavlikova)

Source: JOURNAL OF CHEMICAL INFORMATION AND MODELING **Volume:** 64 **Issue:** 16 **Pages:** 6542-6556 **DOI:** 10.1021/acs.jcim.4c00809 **Early Access Date:** AUG 2024 **Published Date:** 2024 AUG 5

Abstract: By merging advanced dimensionality reduction (DR) and clustering algorithm (CA) techniques, our study advances the sampling procedure for predicting NMR chemical shifts (CS) in intrinsically disordered proteins (IDPs), making a significant leap forward in the field of protein analysis/modeling. We enhance NMR CS sampling by generating clustered ensembles that accurately reflect the different properties and phenomena encapsulated by the IDP trajectories. This investigation critically assessed different rapid CS predictors, both neural network (e.g., Sparta+ and ShiftX2) and database-driven (ProCS-15), and highlighted the need for more advanced quantum calculations and the subsequent need for more tractable-sized conformational ensembles. Although neural network CS predictors outperformed ProCS-15 for all atoms, all tools showed poor agreement with H-N CSs, and the neural network CS predictors were unable to capture the influence of phosphorylated residues, highly relevant for IDPs. This study also addressed the limitations of using direct clustering with collective variables, such as the widespread implementation of the GROMOS algorithm. Clustered ensembles (CEs) produced by this algorithm showed poor performance with chemical shifts compared to sequential ensembles (SEs) of similar size. Instead, we implement a multiscale DR and CA approach and explore the challenges and limitations of applying these algorithms to obtain more robust and tractable CEs. The novel feature of this investigation is the use of solvent-accessible surface area (SASA) as one of the fingerprints for DR alongside previously investigated alpha carbon distance/angles or phi/psi dihedral angles. The ensembles produced with SASA tSNE DR produced CEs better aligned with the experimental CS of between 0.17 and 0.36 r(2) (0.18-0.26 ppm) depending on the system and replicate. Furthermore, this technique produced CEs with better agreement than traditional SEs in 85.7% of all ensemble sizes. This study investigates the quality of ensembles produced based on different input features, comparing latent spaces produced by linear vs nonlinear DR techniques and a novel integrated silhouette score scanning protocol for tSNE DR.

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Record 193 of 274

Title: First-principles guidelines to select promising van der Waals materials for hybrid photovoltaic-triboelectric nanogenerators

Author(s): Cammarata, A (Cammarata, Antonio); Damte, JY (Damte, Jemal Yimer); Polcar, T (Polcar, Tomas)

Source: NANOSCALE **Volume:** 16 **Issue:** 35 **Pages:** 16582-16592 **DOI:** 10.1039/d4nr02217c **Early Access Date:** AUG 2024 **Published Date:** 2024 SEP 12

Abstract: Photovoltaic (PV) devices play a key role in solar-to-electricity energy conversion at small and large scales; unfortunately, their efficiency heavily depends on optimal weather and environmental conditions. The optimal scenario would be to extend the capabilities of PV devices so that they are also able to harvest energy from environmental sources other than light. An optimal solution is represented by hybrid photovoltaic-triboelectric (PV-TENG) devices which have both photovoltaic and triboelectric

capabilities for electric power generation. Two-dimensional transition metal dichalcogenides (TMDs) are highly promising candidates for such PV-TENG devices, thanks to the easy tunability of their electrical, optical, mechanical, and chemical properties. In this respect, we here propose a quantum mechanical study to identify suitable TMD-based chemical compositions with optimal photovoltaic and triboelectric generation properties. Among the considered materials, we identify MoTe2/WS2, MoS2/WSe2, WS2/TiO2, WS2/IrO2, and MoS2/WTe2 as the most promising bilayer compositions; under operative conditions, the band gap varies in the range 0.51-1.61 eV, ensuring the photovoltaic activity, while the relative motion of the layers may produce an electromotive force between 1.21 and 3.21 V (triboelectric generation) with a TMD/TMD interface area equal to about 200 & Aring;2. The results constitute theoretical guidelines on how to check if specific chemical compositions of TMD bilayers are optimal for a combined photovoltaic and triboelectric power generation. Thanks to its generality, the presented approach can be promptly extended to van der Waals heterostructures other than those here considered and implemented in automated workflows for the search of novel low-dimensional materials with target PV and TENG response.
Hybrid photovoltaic-triboelectric nanogenerator (PV-TENG) devices are promising multi-energy harvesters. We provide theoretical guidelines to identify TMD chemical compositions for optimal PV-TENG electric power generation.

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Record 194 of 274

Title: Rational design of MXene-based vacancy-confined single-atom catalyst for efficient oxygen evolution reaction

Author(s): Fu, ZH (Fu, Zhongheng); Hai, GT (Hai, Guangtong); Ma, XX (Ma, Xia-Xia); Legut, D (Legut, Dominik); Zheng, YC (Zheng, Yongchao); Chen, X (Chen, Xiang)

Source: JOURNAL OF ENERGY CHEMISTRY **Volume:** 98 **Pages:** 663-669 **DOI:** 10.1016/j.jechem.2024.07.014 **Early Access Date:** AUG 2024 **Published Date:** 2024 NOV

Abstract: Two-dimensional transition metal carbides (MXenes) have been demonstrated to be promising supports for single-atom catalysts (SACs) to enable efficient oxygen evolution reaction (OER). However, the rational design of MXene-based SACs depends on an experimental trial-and-error approach. A theoretical guidance principle is highly expected for the efficient evaluation of MXene-based SACs. Herein, highthroughput screening was performed through first-principles calculations and machine learning techniques. Ti3C2(OH)x, V3C2(OH)x, Zr3C2(OH)x, Nb3C2(OH)x, Hf3C2(OH)x, Ta3C2(OH)x, and W3C2(OH)x were screened out based on their excellent stability. Zn, Pd, Ag, Cd, Au, and Hg were proposed to be promising single atoms anchored in MXenes based on cohesive energy analysis. Hf3C2(OH)x with a Pd single atom delivers a theoretical overpotential of 81 mV. Both moderate electron-deficient state and high covalency of metal-carbon bonds were critical features for the high OER reactivity. This principle is expected to be a promising approach to the rational design of OER catalysts for metal-air batteries, fuel cells, and other OER-based energy storage devices. (c) 2024 Science Press and Dalian Institute of Chemical Physics, Chinese Academy of Sciences. Published by ELSEVIER B.V. and Science Press.

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Record 195 of 274

Title: The transcriptional landscape of the developmental switch from regular pollen maturation towards microspore-derived plant regeneration in barley

Author(s): Nowicka, A (Nowicka, Anna); Kovacik, M (Kovacik, Martin); Maksylewicz, A (Maksylewicz, Anna); Kopec, P (Kopec, Przemyslaw); Dubas, E (Dubas, Ewa); Krzewska, M (Krzewska, Monika); Springer, A (Springer, Agnieszka); Hoffie, RE (Hoffie, Robert E.); Daghma, DS (Daghma, Diaaeldin S.); Milec, Z (Milec, Zbynek); Pecinka, A (Pecinka, Ales); Kumlehn, J (Kumlehn, Jochen); Zur, I (Zur, Iwona)

Source: CROP JOURNAL **Volume:** 12 **Issue:** 4 **Pages:** 1064-1080 **DOI:** 10.1016/j.cj.2024.07.003 **Published Date:** 2024 AUG

Abstract: Plant formation from in vitro-cultivated microspores involves a complex network of internal and environmental factors. Haploids/doubled haploids (DHs) derived from in vitro-cultured microspores are widely used in plant breeding and genetic engineering. However, the mechanism underlying the developmental switch from regular pollen maturation towards microspore-derived plant regeneration remains poorly defined. Here, RNA-sequencing was employed to elucidate the transcriptional landscapes of four early stages of microspore embryogenesis (ME) in barley cultivars Golden Promise and Igri, which exhibit contrasting responsiveness to microspore-derived plant formation. Our experiments revealed fundamental regulatory networks, specific groups of genes, and transcription factor (TF) families potentially regulating the developmental switch. We identified a set of candidate genes crucial for genotype-dependent responsiveness/recalcitrance to ME. Our high-resolution temporal transcriptome atlas provides an important resource for future functional studies on the genetic control of microspore developmental transition. (c) 2024 Crop Science Society of China and Institute of Crop Science, CAAS. Production and hosting by Elsevier B.V. on behalf of KeAi Communications Co., Ltd. This is an open access article under the CC BY-NCND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

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Record 196 of 274

Title: Positron unveiling high mobility graphene stack interfaces in Li-ion cathodes

Author(s): Zheng, MY (Zheng, Meiying); Kuriplach, J (Kuriplach, Jan); Makkonen, I (Makkonen, Ilja); Ferragut, R (Ferragut, Rafael); Di Noto, V (Di Noto, Vito); Pagot, G (Pagot, Gioele); Laakso, E (Laakso, Ekaterina); Barbiellini, B (Barbiellini, Bernardo)

Source: COMMUNICATIONS MATERIALS **Volume:** 5 **Issue:** 1 **Article Number:** 138 **DOI:** 10.1038/s43246-024-00561-w **Published Date:** 2024 JUL 27

Abstract: Carbon-based coatings in Li-ion battery cathodes improve electron conductivity and enable rapid charging. However, the mechanism is not well understood. Here, we address this question by using positrons as non-destructive probes to investigate nano-interfaces within cathodes. We calculate the positron annihilation lifetime in a graphene stack LiCoO2 heterojunction using an ab initio method with a non-local density approximation to accurately describe the electron-positron correlation. This ideal heterostructure represents the standard carbon-based coating performed on cathode nanoparticles to improve the conduction properties of the cathode. We characterize the interface between LiCoO2 and graphene as a p-type Schottky junction and find positron surface states. The intensity of the lifetime component for these positron surface states serves as a descriptor for positive ion ultra-fast mobility. Consequently, optimizing the carbon layer by enhancing this intensity and by analogizing Li-ion adatoms on graphene layers with positrons at surfaces can improve the design of fast-charging channels.
Carbon layers in Li-ion battery cathodes are important for fast charging but the underlying mechanism is still not well understood. Here, ab initio calculations of the positron annihilation lifetime in graphene stack LiCoO2 heterojunction gives insights into ultra-fast ion mobility.

Accession Number: WOS:001280874800001

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eISSN: 2662-4443

Record 197 of 274

Title: Deeper Insight of the Conformational Ensemble of Intrinsically Disordered Proteins

Author(s): Svensson, O (Svensson, Oskar); Bakker, MJ (Bakker, Michael J.); Skepö, M (Skepo, Marie)

Source: JOURNAL OF CHEMICAL INFORMATION AND MODELING **Volume:** 64 **Issue:** 15 **Pages:** 6105-6114 **DOI:** 10.1021/acs.jcim.4c00941 **Early Access Date:** JUL 2024 **Published Date:** 2024 JUL 26

Abstract: It is generally known that, unlike structured proteins, intrinsically disordered proteins, IDPs, exhibit various structures and conformers, the so-called conformational ensemble, CoE. This study aims to better understand the conformers that make up the IDP ensemble by decomposing the CoE into groups separated by their radius of gyration, R-g. A common approach to studying CoE for IDPs is to use low-resolution techniques, such as small-angle scattering, and combine those with computer simulations on different length scales. Herein, the well-studied antimicrobial saliva protein histatin 5 was utilized as a model peptide for an IDP; the average intensity curves were obtained from small-angle X-ray scattering;

and compared with fully atomistic, explicit water, molecular dynamics simulations; then, the intensity curve was decomposed with respect to the different R-g values; and their secondary structure propensities were investigated. We foresee that this approach can provide important information on the CoE and the individual conformers within; in that case, it will serve as an additional tool for understanding the IDP structure-function relationship on a more detailed level.

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PubMed ID: 39056166

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Record 198 of 274

Title: Corruption dynamics in public procurement: A longitudinal network analysis of local construction contracts in Guatemala

Author(s): Waxenecker, H (Waxenecker, Harald); Prell, C (Prell, Christina)

Source: SOCIAL NETWORKS **Volume:** 79 **Pages:** 154-167 **DOI:** 10.1016/j.socnet.2024.07.001 **Early Access Date:** JUL 2024 **Published Date:** 2024 OCT

Abstract: Spending concentration, political influence, and collusion violate rules and principles of open and fair public procurement, leading to corrupt contract allocation. This study adopts stochastic actor-oriented models to test the evolution of these forms of procurement corruption risks in a longitudinal network study of 33579 construction contracts pertaining to Guatemalan local governments from 2012 to 2020. We identify a range of network configurations, based on past empirical research and theory, that capture different patterns of suspicious micro tendencies suggestive of corruption. We show how these micro tendencies shift in strength according to changes in electoral cycles and anti-corruption interventions, thus shedding light on how interventions may temporarily impact corrupt behavior, and how it may adapt and persist after a period of transition. The results indicate that collusion and spending concentration play significant roles in sustaining the risk of corrupt contract allocation, and that this behavior is able to rebound even after the introduction of anti-corruption interventions and new political regimes. The findings underscore the importance of local interventions and advocate for network approaches to enhance transparency, accountability, and long-term anti-corruption efforts.

Accession Number: WOS:001281511300001

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Record 199 of 274

Title: An approach for dynamically adaptable SIMD vectorization of FEM kernels

Author(s): Kadlubiak, K (Kadlubiak, Kristian); Meca, O (Meca, Ondrej); Říha, L (Riha, Lubomir); Brzobohaty, T (Brzobohaty, Tomas)

Source: COMPUTER PHYSICS COMMUNICATIONS **Volume:** 304 **Article Number:** 109319 **DOI:** 10.1016/j.cpc.2024.109319 **Early Access Date:** JUL 2024 **Published Date:** 2024 NOV

Abstract: The paper focuses on the optimization of the FEM matrix kernels with respect to user-defined parameters such as materials, initial conditions, and boundary conditions that are known during run-time only. Adapting the kernels to specific parameters can save a significant amount of execution time and increase performance. Handling them efficiently is challenging due to the exponential number of potential combinations that the user can specify. The paper presents an approach that combines (a) cross-element vectorization for the easy-to-write transformation of the original scalar code to vectorized one, (b) meta-programming for utilization of a compiler for building sub- kernels tailored for a particular set of parameters, (c) and dynamic polymorphism allowing run-time selection of sub-kernels. We show that the above techniques allow (1) straightforward code modifications, (2) efficient handling of required dynamic behavior with a minor performance penalty for most kernels, and (3) achieving up to 8-fold speedups compared to non-adapted kernels.

Accession Number: WOS:001279658300001

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Record 200 of 274

Title: Identifying type II quasars at intermediate redshift with few-shot learning photometric classification

Author(s): Cunha, PAC (Cunha, P. A. C.); Humphrey, A (Humphrey, A.); Brinchmann, J (Brinchmann, J.); Morais, SG (Morais, S. G.); Carvajal, R (Carvajal, R.); Gomes, JM (Gomes, J. M.); Matute, I (Matute, I.); Paulino-Afonso, A (Paulino-Afonso, A.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 687 **Article Number:** A269 **DOI:** 10.1051/0004-6361/202346426 **Published Date:** 2024 JUL 23

Abstract: Context. A sub-population of AGNs where the central engine is obscured are known as type II quasars (QSO2s). These luminous AGNs have a thick and dusty torus that obscures the accretion disc from our line of sight. Thus, their special orientation allows for detailed studies of the AGN-host co-evolution. Increasing the sample size of QSO2 sources in critical redshift ranges is crucial for understanding the interplay of AGN feedback, the AGN-host relationship, and the evolution of active galaxies.
Aims. We aim to identify QSO2 candidates in the 'redshift desert' using optical and infrared photometry. At this intermediate redshift range (i.e. 1 <= z <= 2), most of the prominent optical emission lines in QSO2 sources (e.g. CIV lambda l549; [OIII]lambda lambda 4959, 5008) fall either outside the wavelength range of the SDSS optical spectra or in particularly noisy wavelength ranges, making QSO2 identification challenging. Therefore, we adopted a semi-supervised machine learning approach to select candidates in the SDSS galaxy sample.
Methods. Recent applications of machine learning in astronomy focus on problems involving large data sets, with small data sets often being overlooked. We developed a 'few-shot' learning approach for the identification and classification of rare-object classes using limited training data (200 sources). The new AMELIA pipeline uses a transfer-learning based approach with decision trees, distance-based, and deep learning methods to build a classifier capable of identifying rare objects on the basis of an observational training data set.
Results. We validated the performance of AMELIA by addressing the problem of identifying QSO2s at 1 <= z <= 2 using SDSS and WISE photometry, obtaining an F1-score above 0.8 in a supervised approach. We then used AMELIA to select new QSO2 candidates in the 'redshift desert' and examined the nature of the candidates using SDSS spectra, when available. In particular, we identified a sub-population of

[NeV]lambda 3426 emitters at z similar to 1.1, which are highly likely to contain obscured AGNs. We used X-ray and radio crossmatching to validate our classification and investigated the performance of photometric criteria from the literature showing that our candidates have an inherent dusty nature. Finally, we derived physical properties for our QSO2 sample using photoionisation models and verified the AGN classification using an SED fitting.
Conclusions. Our results demonstrate the potential of few-shot learning applied to small data sets of rare objects, in particular QSO2s, and confirms that optical-IR information can be further explored to search for obscured AGNs. We present a new sample of candidates to be further studied and validated using multi-wavelength observations.

Accession Number: WOS:001275047000004

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ISSN: 0004-6361

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Record 201 of 274

Title: Azobenzene-Based Photoswitchable Substrates for Advanced Mechanistic Studies of Model Haloalkane Dehalogenase Enzyme Family

Author(s): Slanska, M (Slanska, Michaela); Stackova, L (Stackova, Lenka); Marques, SM (Marques, Sergio M.); Stacko, P (Stacko, Peter); Martínek, M (Martinek, Marek); Jílek, L (Jilek, Lubos); Toul, M (Toul, Martin); Damborsky, J (Damborsky, Jiri); Bednar, D (Bednar, David); Klán, P (Klan, Petr); Prokop, Z (Prokop, Zbynek)

Source: ACS CATALYSIS **Volume:** 14 **Issue:** 15 **Pages:** 11635-11645 **DOI:** 10.1021/acscatal.4c03503 **Early Access Date:** JUL 2024 **Published Date:** 2024 JUL 22

Abstract: The engineering of efficient enzymes for large-scale production of industrially relevant compounds is a challenging task. Utilizing rational protein design, which relies on a comprehensive understanding of mechanistic information, holds significant promise for achieving success in this endeavor. Pre-steady-state kinetic measurements, obtained either through fast-mixing techniques or photoswitchable substrates, provide crucial mechanistic insights. The latter approach not only furnishes mechanistic clarity but also affords real-time structural elucidation of reaction intermediates via time-resolved femtosecond crystallography. Unfortunately, only a limited number of such valuable mechanistic probes are available. To address this gap, we applied a multidisciplinary approach, including computational analysis, chemical synthesis, physicochemical property screening, and enzyme kinetics to identify promising candidates for photoswitchable probes. We demonstrate the approach by designing an azobenzene-based photoswitchable substrate tailored for haloalkane dehalogenases, a prototypic class of enzymes pivotal in developing computational tools for rational protein design. The probe was subjected to steady-state and pre-steady-state kinetic analysis, which revealed new insights about the catalytic behavior of the model biocatalysts. We employed laser-triggered Z-to-E azobenzene photoswitching to generate the productive isomer in situ, opening avenues for advanced mechanistic studies using time-resolved femtosecond crystallography. Our results not only pave the way for the mechanistic understanding of this model enzyme family, incorporating both kinetic and structural dimensions, but also propose a systematic approach to the rational design of photoswitchable enzymatic substrates.

Accession Number: WOS:001274503900001

PubMed ID: 39114093

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ISSN: 2155-5435

Record 202 of 274

Title: Handling simulation failures of a computationally expensive multiobjective optimization problem in pump design

Author(s): Mazumdar, A (Mazumdar, Atanu); Burkotová, J (Burkotova, Jana); Krátky, T (Kratky, Tomas); Chugh, T (Chugh, Tinkle); Miettinen, K (Miettinen, Kaisa)

Source: ENGINEERING APPLICATIONS OF ARTIFICIAL INTELLIGENCE **Volume:** 136 **Article Number:** 108897 **DOI:** 10.1016/j.engappai.2024.108897 **Early Access Date:** JUL 2024 **Published Date:** 2024 OCT **Part:** A

Abstract: Solving real-world optimization problems in engineering and design involves various practical challenges. They include simultaneously optimizing multiple conflicting objective functions that may involve computationally expensive simulations. Failed simulations introduce another practical challenge, as it is not always possible to set constraints a priori to avoid failed simulations. Failed simulations are typically ignored during optimization, which leads to wasting computation resources. When the optimization problem has multiple objective functions, failed simulations can also be misleading for the decision maker while choosing the most preferred solution. Utilizing data collected from previous simulations and enabling the optimization algorithm to avoid failed simulations can reduce the computational requirements. We consider data-driven multiobjective optimization of the diffusor of an axial pump and propose an approach to reduce the number of solutions that fail in expensive computational fluid dynamics simulations. The proposed approach utilizes Kriging surrogate models to approximate the objective functions and is inexpensive to evaluate. We utilize a probabilistic selection approach with constraints in a multiobjective evolutionary algorithm to find solutions with better objective function values, lower uncertainty, and lower probability of failing. Finally, a domain expert chooses the most preferred solution using one's preferences. Numerical tests show significant improvement in the ratio of feasible solutions to all the available solutions without special treatment of failed simulations. The solutions also have a higher quality (hypervolume) and accuracy than the other tested approaches. The proposed approach provides an efficient way of reducing the number of failed simulations and utilizing offline data in multiobjective design optimization.

Accession Number: WOS:001270782600001

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Record 203 of 274

Title: Solving linear and nonlinear problems using Taylor series method

Author(s): Veigend, P (Veigend, Petr); Necasová, G (Necasova, Gabriela); Sátek, V (Satek, Vaclav)

Source: OPEN COMPUTER SCIENCE **Volume:** 14 **Issue:** 1 **Article Number:** 20240005 **DOI:** 10.1515/comp-2024-0005 **Published Date:** 2024 JUL 12

Abstract: The article deals with the solution of technical initial value problems. To solve such problems, an analytical or numerical approach is possible. The analytical approach can provide an accurate result; however, it is not available for all problems and it is not entirely suitable for calculation on a computer, due to the limited numerical accuracy. For this reason, the numerical approach is preferred. This approach uses ordinary differential equations to approximate the continuous behaviour of the real-world system. There are many known numerical methods for solving such equations, most of them limited in their accuracy, have a limited region of stability and can be quite slow to achieve the acceptable solution. The numerical method proposed in this article is based on the Taylor series and overcomes the biggest challenge, i.e. calculating higher derivatives. The aim of the article is therefore twofold: to introduce the method and show its properties, and to show its behaviour when solving problems composed of linear and nonlinear ordinary differential equations. Linear problems are modelled by partial differential equations and solved in parallel using the PETSc library. The parallel solution is demonstrated using the wave equation, which is transformed into the system of ordinary differential equations using the method of lines. The solution of nonlinear problems is introduced together with several optimisations that significantly increase the calculation speed. The improvements are demonstrated using several numerical examples that are solved using MATLAB software.

Accession Number: WOS:001270179500001

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Record 204 of 274

Title: Chemical space exploration with Molpher: Generating and assessing a glucocorticoid receptor ligand library

Author(s): Agea, MI (Agea, M. Isabel); Cmelo, I (Cmelo, Ivan); Dehaen, W (Dehaen, Wim); Chen, Y (Chen, Ya); Kirchmair, J (Kirchmair, Johannes); Sedlak, D (Sedlak, David); Bartunek, P (Bartunek, Petr); Sícho, M (Sicho, Martin); Svozil, D (Svozil, Daniel)

Source: MOLECULAR INFORMATICS **Volume:** 43 **Issue:** 8 **DOI:** 10.1002/minf.202300316 **Early Access Date:** JUL 2024 **Published Date:** 2024 AUG

Abstract: Computational exploration of chemical space is crucial in modern cheminformatics research for accelerating the discovery of new biologically active compounds. In this study, we present a detailed analysis of the chemical library of potential glucocorticoid receptor (GR) ligands generated by the molecular generator, Molpher. To generate the targeted GR library and construct the classification models, structures from the ChEMBL database as well as from the internal IMG library, which was experimentally screened for biological activity in the primary luciferase reporter cell assay, were utilized. The composition of the targeted GR ligand library was compared with a reference library that randomly samples chemical space. A random forest model was used to determine the biological activity of ligands, incorporating its applicability domain using conformal prediction. It was demonstrated that the GR library is significantly enriched with GR ligands compared to the random library. Furthermore, a prospective analysis demonstrated that Molpher successfully designed compounds, which were subsequently experimentally confirmed to be active on the GR. A collection of 34 potential new GR ligands was also identified. Moreover, an important contribution of this study is the establishment of a

comprehensive workflow for evaluating computationally generated ligands, particularly those with potential activity against targets that are challenging to dock.
In this study, it was demonstrated that the molecular generator, Molpher, significantly enriches the chemical library with glucocorticoid receptor (GR) ligands compared to a random library. Utilizing the ChEMBL and IMG internal library of bioactive compounds, 34 potential new GR ligands were identified, and a comprehensive workflow for evaluating computationally generated ligands was established. image

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PubMed ID: 38979783

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ISSN: 1868-1743

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Record 205 of 274

Title: La₂C₂@D₅(450)-C₁₀₀: Calculated High Energy Gain in Encapsulation

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

Source: INORGANICS **Volume:** 12 **Issue:** 7 **Article Number:** 196 **DOI:** 10.3390/inorganics12070196 **Published Date:** 2024 JUL

Abstract: The structure and energetics of the clusterfullerene La2C2@D-5(450)-C-100 are calculated at the B3LYP/6-31G*similar to SDD level (including counterpoise correction for the basis set superposition error), and the observed features are confirmed. Its stability is explained by substantial energy gain connected with the encapsulation, viz. 140 kcal/mol per atom of the encapsulate, actually higher than previously found for comparable systems.

Accession Number: WOS:001278815200001

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Record 206 of 274

Title: Ir(I)-Bi(III) Donor-Acceptor Adducts Stabilized by Dispersion Interactions between the Metal Pincer Ligands and Their Possible Self-Assembly Forming Molecular 1D Semiconductors

Author(s): Chval, Z (Chval, Zdenek)

Source: INORGANIC CHEMISTRY **Volume:** 63 **Issue:** 27 **Pages:** 12417-12425 **DOI:** 10.1021/acs.inorgchem.4c00364 **Early Access Date:** JUN 2024 **Published Date:** 2024 JUN 26

Abstract: Structure, stability, and electronic properties of the bimetallic {[Ir-I(terpy)(Me)]-[(BiNNN)-N-III]} n monomeric, oligomeric, and polymeric structures (n = 1-3 and infinity; terpy = terpyridine; Me = methyl; BiNNN = bismuth triamide) and their derivatives (designated as (Bi<middle dot>Ir)(n) structures) were studied theoretically by DFT cluster and periodic calculations. Stable Bi<middle dot>Ir adducts (monomers) were formed with short Bi-Ir bonds (<2.7 & Aring;) and Gibbs free binding energies larger than 20 kcal/mol for all systems. The substitution of the pincer ligands of Ir(I) and Bi(III) complexes by the electron-donating (NH2) and electron-withdrawing (NO2, F, CF3) groups, respectively, enhanced the Ir -> Bi charge transfer, substantially stabilizing the Bi<middle dot>Ir monomers. The monomers from the unsubstituted complexes can be considered as dispersion stabilized adducts, and they may form spontaneously (Bi<middle dot>Ir)(n) layered oligomers/polymers with semiconducting properties. The self-assembly of monomers into oligomers/polymers is hindered by bulkier protecting groups on the Bi(III) complex, such as tBu and SiMe3.

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PubMed ID: 38923937

Author Identifiers:

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ISSN: 0020-1669

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Record 207 of 274

Title: Analysis of striatal connectivity corresponding to striosomes and matrix in de novo Parkinson's disease and isolated REM behavior disorder

Author(s): Marecek, S (Marecek, S.); Krajca, T (Krajca, T.); Krupicka, R (Krupicka, R.); Sojka, P (Sojka, P.); Nepozitek, J (Nepozitek, J.); Varga, Z (Varga, Z.); Mala, C (Mala, C.); Keller, J (Keller, J.); Waugh, JL (Waugh, J. L.); Zogala, D (Zogala, D.); Trnka, J (Trnka, J.); Sonka, K (Sonka, K.); Ruzicka, E (Ruzicka, E.); Dusek, P (Dusek, P.)

Source: NPJ PARKINSONS DISEASE **Volume:** 10 **Issue:** 1 **Article Number:** 124 **DOI:** 10.1038/s41531-024-00736-9 **Published Date:** 2024 JUN 25

Abstract: Striosomes and matrix are two compartments that comprise the striatum, each having its own distinct immunohistochemical properties, function, and connectivity. It is currently not clear whether prodromal or early manifest Parkinson's disease (PD) is associated with any striatal matrix or striosomal abnormality. Recently, a method of striatal parcellation using probabilistic tractography has been described and validated, using the distinct connectivity of these two compartments to identify voxels with striosome- and matrix-like connectivity. The goal of this study was to use this approach in tandem with DAT-SPECT, a method used to quantify the level of nigrostriatal denervation, to analyze the striatum in populations of de novo diagnosed, treatment-na & iuml;ve patients with PD, isolated REM behavioral disorder (iRBD) patients, and healthy controls. We discovered a shift in striatal connectivity, which showed correlation with nigrostriatal denervation. Patients with PD exhibited a significantly higher matrix-like volume and associated connectivity than healthy controls and higher matrix-associated connectivity than iRBD patients. In contrast, the side with less pronounced nigrostriatal denervation in PD and iRBD patients showed a decrease in striosome-like volume and associated connectivity indices. These findings could point to a compensatory neuroplastic mechanism in the context of nigrostriatal denervation and open a new avenue in the investigation of the pathophysiology of Parkinson's disease.

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PubMed ID: 38918417

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eISSN: 2373-8057

Record 208 of 274

Title: The role of defects in high-silica zeolite hydrolysis and framework healing

Author(s): Liu, MX (Liu, Mingxiu); Grajciar, L (Grajciar, Lukas); Heard, CJ (Heard, Christopher J.)

Source: MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 377 **Article Number:** 113219 **DOI:** 10.1016/j.micromeso.2024.113219 **Early Access Date:** JUN 2024 **Published Date:** 2024 SEP

Abstract: The stability of high silica zeolites under standard laboratory and mild steaming conditions is understood to be due to the lack of hydrophilic Al-O-Si moieties, which can be targeted by water via hydrolysis reactions with relatively low barriers. However, in hydrophobic high-silica and siliceous frameworks, the specific interactions between water and the internal framework sites are incompletely understood. In particular, the behaviour of common internal defects, including partial hydrolysis species and silanol nests are not established, despite their expected role in accelerating the decomposition of the framework. In this work, we utilise machine learning potentials combined with density functional calculations to rigorously sample the hydrolysis processes in siliceous zeolites with topologies CHA and MFI under low water conditions and quantify the effect of defects. Internal silanol defect sites are found to accelerate zeolite decomposition primarily by bypassing the initial, highbarrier hydrolysis step. Subsequent steps proceed with lower reaction barriers. However, all reaction steps are found to be highly activated, and unlikely to occur rapidly at room temperature under conditions of low internal water concentration. Exchange-healing routes, which reverse hydrolysis while incorporating oxygen from water molecules are found to be competitive along the entire hydrolysis pathway in CHA, providing an additional source of stabilization against hydrolytic decomposition.

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Record 209 of 274

Title: Subclinical peripheral inflammation has systemic effects impacting central nervous system proteome in budgerigars

Author(s): Voukali, E (Voukali, Eleni); Divín, D (Divin, Daniel); Samblas, MG (Samblas, Mercedes Gomez); Veetil, NK (Veetil, Nithya Kuttiyarthu); Krajzingrová, T (Krajzingrova, Tereza); Tesicky, M (Tesicky, Martin); Li, T (Li, Tao); Melepat, B (Melepat, Balraj); Talacko, P (Talacko, Pavel); Vinkler, M (Vinkler, Michal)

Source: DEVELOPMENTAL AND COMPARATIVE IMMUNOLOGY **Volume:** 159 **Article Number:** 105213 **DOI:** 10.1016/j.dci.2024.105213 **Early Access Date:** JUN 2024 **Published Date:** 2024 OCT

Abstract: Regulation of neuroimmune interactions varies across avian species. Little is presently known about the interplay between periphery and central nervous system (CNS) in parrots, birds sensitive to neuroinflammation. Here we investigated the systemic and CNS responses to dextran sulphate sodium (DSS)- and lipopolysaccharide (LPS)induced subclinical acute peripheral inflammation in budgerigar (Melopsittacus undulatus). Three experimental treatment groups differing in DSS and LPS stimulation were compared to controls. Individuals treated with DSS showed significant histological intestinal damage. Through quantitative proteomics we described changes in plasma (PL) and cerebrospinal fluid (CSF) composition. In total, we identified 180 proteins in PL and 978 proteins in CSF, with moderate co - structure between the proteomes. Between treatments we detected differences in immune, coagulation and metabolic pathways. Proteomic variation was associated with the levels of proinflammatory cytokine mRNA expression in intestine and brain. Our findings shed light on systemic impacts of peripheral low-grade inflammation in birds.

Accession Number: WOS:001258278300001

PubMed ID: 38880215

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Voukali, Eleni	M-5082-2018	
Tesicky, Martin	L-3370-2017	
Melepat, Balraj	AAQ-5774-2021	
Kuttiyarthu Veetil, Nithya	KBB-0262-2024	
Talacko, Pavel	H-8921-2017	
Melepat, Balraj		0000-0002-1830-9124
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Divin, Daniel		0000-0001-8513-7214
Voukali, Eleni		0000-0001-6029-6171

ISSN: 0145-305X

eISSN: 1879-0089

Record 210 of 274

Title: Contributions beyond direct random-phase approximation in the binding energy of solid ethane, ethylene, and acetylene

Author(s): Pham, KN (Pham, Khanh Ngoc); Modrzejewski, M (Modrzejewski, Marcin); Klimes, J (Klimes, Jiri)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 160 **Issue:** 22 **Article Number:** 224101 **DOI:** 10.1063/5.0207090 **Published Date:** 2024 JUN 14

Abstract: The random-phase approximation (RPA) includes a subset of higher than second-order correlation-energy contributions, but stays in the same complexity class as the second-order Moller-Plesset perturbation theory (MP2) in both Gaussian-orbital and plane-wave codes. This makes RPA a promising ab initio electronic structure approach for the binding energies of molecular crystals. Still, some issues stand out in practical applications of RPA. Notably, compact clusters of nonpolar molecules are poorly described, and the interaction energies strongly depend on the reference single-determinant state. Using the many-body expansion of the binding energy of a crystal, we investigate those issues and

the effect of beyond-RPA corrections. We find the beneficial effect of quartic-scaling exchange and non-ring coupled-cluster doubles corrections. The nonadditive interactions in compact trimers of molecules are improved by using the self-consistent Hartree-Fock orbitals instead of the usual Kohn-Sham states, but this kind of orbital input also leads to underestimated dimer energies. Overall, a substantial improvement over the RPA with a renormalized singles approach is possible at a modest quartic-scaling cost, which encourages further research into additional RPA corrections.

Accession Number: WOS:001244483600006

PubMed ID: 38856055

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Modrzejewski, Marcin	HGE-3832-2022	
Klimes, Jiri	D-8926-2011	0000-0003-4969-1343

ISSN: 0021-9606

eISSN: 1089-7690

Record 211 of 274

Title: Phosphorylation site of L-alanyl-L-glutamine identified by Raman optical activity spectroscopy

Author(s): Wu, T (Wu, Tao); Kessler, J (Kessler, Jiri); Zhao, H (Zhao, Hua); Zhao, YF (Zhao, Yufen)

Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 320 **Article Number:** 124587 **DOI:** 10.1016/j.saa.2024.124587 **Early Access Date:** JUN 2024 **Published Date:** 2024 NOV 5

Abstract: Phosphorylated peptides are instrumental in studying protein phosphorylation events. In the present study, Raman optical activity (ROA) is employed to elucidate the structure of a dipeptide, L-alanyl-L-glutamine (L-AlaL-Gln) and its two differently alkylated N -phosphorylated derivatives. Theoretical simulations were conducted to aid the interpretation of peptide conformation variations upon phosphorylation, and of the measured Raman and ROA spectra. Induced circularly polarized luminescence (CPL) was also recorded in solution, in the presence of a simple europium aqua ion. As the spectra are peptide specific, this type of stereochemical analysis is expected to aid identification of the phosphorylation sites also in other peptides and possibly proteins.

Accession Number: WOS:001251417200001

PubMed ID: 38850816

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kessler, Jiří	G-2880-2012	
Wu, Tao	B-3667-2010	0000-0002-0244-3046

ISSN: 1386-1425

eISSN: 1873-3557

Record 212 of 274

Title: Investigating the effects of radiation, T cell depletion, and bone marrow transplantation on murine gut microbiota

Author(s): Kreisinger, J (Kreisinger, Jakub); Dooley, J (Dooley, James); Singh, K (Singh, Kailash); Cizková, D (Cizkova, Dagmar); Schmiedová, L (Schmiedova, Lucie); Bendová, B (Bendova, Barbora); Liston, A (Liston, Adrian); Moudra, A (Moudra, Alena)

Source: FRONTIERS IN MICROBIOLOGY **Volume:** 15 **Article Number:** 1324403 **DOI:** 10.3389/fmicb.2024.1324403 **Published Date:** 2024 JUN 5

Abstract: Microbiome research has gained much attention in recent years as the importance of gut microbiota in regulating host health becomes increasingly evident. However, the impact of radiation on the microbiota in the murine bone marrow transplantation model is still poorly understood. In this paper, we present key findings from our study on how radiation, followed by bone marrow transplantation with or without T cell depletion, impacts the microbiota in the ileum and caecum. Our findings show that radiation has different effects on the microbiota of the two intestinal regions, with the caecum showing increased interindividual variation, suggesting an impaired ability of the host to regulate microbial symbionts, consistent with the Anna Karenina principle. Additionally, we observed changes in the ileum composition, including an increase in bacterial taxa that are important modulators of host health, such as Akkermansia and Faecalibaculum. In contrast, radiation in the caecum was associated with an increased abundance of several common commensal taxa in the gut, including Lachnospiraceae and Bacteroides. Finally, we found that high doses of radiation had more substantial effects on the caecal microbiota of the T-cell-depleted group than that of the non-T-cell-depleted group. Overall, our results contribute to a better understanding of the complex relationship between radiation and the gut microbiota in the context of bone marrow transplantation and highlight the importance of considering different intestinal regions when studying microbiome responses to environmental stressors.

Accession Number: WOS:001249151300001

PubMed ID: 38903788

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kreisinger, Jakub	H-4020-2011	
Cizkova, Dagmar	KEH-9336-2024	
Moudra, Alena	S-1833-2017	0000-0003-3465-7812
Schmiedova, Lucie	S-3351-2017	0000-0003-2180-5281

eISSN: 1664-302X

Record 213 of 274

Title: Dynamics of Coordinated Phosphonate Group Directly Observed by ¹⁷O-NMR in Lanthanide(III) Complexes of a Mono(ethyl phosphonate) DOTA Analogue

Author(s): Svítok, A (Svitok, Adam); Blahut, J (Blahut, Jan); Urbanovsky, P (Urbanovsky, Peter); Hermann, P (Hermann, Petr)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 30 **Issue:** 36 **DOI:** 10.1002/chem.202400970 **Early Access Date:** JUN 2024 **Published Date:** 2024 JUN 25

Abstract: Biological phosphates can coordinate metal ions and their complexes are common in living systems. Dynamics of mutual oxygen atom exchange in the tetrahedral group in complexes has not been investigated. Here, we present a direct experimental proof of exchange ("phosphonate rotation") in model Ln(III) complexes of monophosphonate H(4)dota analogue which alters phosphorus atom chirality of coordinated phosphonate monoester. Combination of macrocycle-based isomerism with P-based chirality leads to several diastereoisomers. (Non)-coordinated oxygen atoms were distinguished through O-17-labelled phosphonate group and their mutual exchange was followed by various NMR techniques and DFT calculations. The process is sterically demanding and occurs through bulky bidentate (kappa(2)-PO2)(-) coordination and was observed only in twisted-square antiprism (TSA) diastereoisomer of large Ln(III) ions. Its energy demands increase for smaller Ln(III) ions ((298)Delta G(not equal)(exp./DFT)=51.8/52.1 and 61.0/71.5 kJ mol(-1) for La(III) and Eu(III), respectively). These results are helpful in design of such complexes as MRI CA and for protein paramagnetic NMR probes. It demonstrates usefulness of O-17 NMR to study solution dynamics in complexes involving phosphorus acid derivatives and it may inspire use of this method to study dynamics of phosphoric acid derivatives (as e. g. phosphorus acid-based inhibitors of metalloenzymes) in different areas of chemistry.

Accession Number: WOS:001239455700001

PubMed ID: 38624256

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Blahut, Jan	B-2073-2017	0000-0001-7752-8370
Hermann, Petr	A-1880-2008	0000-0001-6250-5125
Svitok, Adam	KVC-1977-2024	0009-0000-4723-2034

ISSN: 0947-6539

eISSN: 1521-3765

Record 214 of 274

Title: Optimal Scanning Pattern for Initial Free-Space Optical-Link Alignment

Author(s): Skryja, P (Skryja, Petr); Barcik, P (Barcik, Peter)

Source: PHOTONICS **Volume:** 11 **Issue:** 6 **Article Number:** 540 **DOI:** 10.3390/photonics11060540 **Published Date:** 2024 JUN

Abstract: Since free-space optical links (especially fully photonic ones) are very challenging to accurately align; scanning algorithms are used for the initial search and alignment of the transceivers. The initial alignment aims to intercept the optical beam so that it hits a position-sensitive detector. However, this operation can be very time-consuming (depending on the system parameters, such as transceiver parameters, distance between transceivers, divergence of the transmitter, angle of view of the receiver, etc.). A spiral scan is used as the most widespread pattern for scanning. This article examines the effects of system parameters (e.g., global navigation satellite systems and compass accuracy) on the angular area of uncertainty that must be scanned to find the optical beam. Furthermore, several types of spiral pattern are compared depending on the time of the scan execution and the required number of points for scanning the given uncertainty area. The cut hexagonal spiral scan achieved the best results as it required 18.1% less time than the common spiral scan for the presented transceiver.

Accession Number: WOS:001256455900001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Skryja, Petr	KPY-4999-2024	0009-0008-9399-2884
Barcik, Peter	G-1724-2019	0000-0002-3922-3979

eISSN: 2304-6732

Record 215 of 274

Title: The strength of gut microbiota transfer along social networks and genealogical lineages in the house mouse

Author(s): Bendová, B (Bendova, Barbora); Bimová, BV (Bimova, Barbora Voslajerova); Cizková, D (Cizkova, Dagmar); Daniszová, K (Daniszova, Kristina); Dureje, L (Dureje, Ludovit); Hiadlovská, Z (Hiadlovska, Zuzana); Macholán, M (Macholan, Milos); Piálek, J (Pialek, Jaroslav); Schmiedová, L (Schmiedova, Lucie); Kreisinger, J (Kreisinger, Jakub)

Source: FEMS MICROBIOLOGY ECOLOGY **Volume:** 100 **Issue:** 6 **Article Number:** fiae075 **DOI:** 10.1093/femsec/fiae075 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 14

Abstract: The gut microbiota of vertebrates is acquired from the environment and other individuals, including parents and unrelated conspecifics. In the laboratory mouse, a key animal model, inter-individual interactions are severely limited and its gut microbiota is abnormal. Surprisingly, our understanding of how inter-individual transmission impacts house mouse gut microbiota is solely derived from laboratory experiments. We investigated the effects of inter-individual transmission on gut microbiota in two subspecies of house mice (Mus musculus musculus and M. m. domesticus) raised in a semi-natural environment without social or mating restrictions. We assessed the correlation between microbiota composition (16S rRNA profiles), social contact intensity (microtransponder-based social

networks), and mouse relatedness (microsatellite-based pedigrees). Inter-individual transmission had a greater impact on the lower gut (colon and cecum) than on the small intestine (ileum). In the lower gut, relatedness and social contact independently influenced microbiota similarity. Despite female-biased parental care, both parents exerted a similar influence on their offspring's microbiota, diminishing with the offspring's age in adulthood. Inter-individual transmission was more pronounced in M. m. domesticus, a subspecies, with a social and reproductive network divided into more closed modules. This suggests that the transmission magnitude depends on the social and genetic structure of the studied population.
The influence of social contacts and relatedness on microbiota is greater in cecum and colon than in ileum; fathers and mothers have a comparable influence on microbiota of the offspring.

Accession Number: WOS:001233917100001

PubMed ID: 38730559

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kreisinger, Jakub	H-4020-2011	
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Piálek, Jaroslav	AAP-8636-2020	
Daniszova, Kristina	JMP-9288-2023	
Hiadlovska, Zuzana	G-7192-2014	
Cizkova, Dagmar		0000-0001-5031-7792
Schmiedova, Lucie	S-3351-2017	0000-0003-2180-5281
Macholan, Milos		0000-0001-5663-6831
Hiadlovska, Zuzana		0000-0003-4730-4557
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Pialek, Jaroslav		0000-0002-0829-7481
Kreisinger, Jakub		0000-0001-9375-9814

ISSN: 0168-6496

eISSN: 1574-6941

Record 216 of 274

Title: Insight into chromatin compaction and spatial organization in rice interphase nuclei

Author(s): Dolezalová, A (Dolezalova, Alzbeta); Beránková, D (Berankova, Denisa); Kolácková, V (Kolackova, Veronika); Hribová, E (Hribova, Eva)

Source: FRONTIERS IN PLANT SCIENCE **Volume:** 15 **Article Number:** 1358760 **DOI:** 10.3389/fpls.2024.1358760 **Published Date:** 2024 MAY 28

Abstract: Chromatin organization and its interactions are essential for biological processes, such as DNA repair, transcription, and DNA replication. Detailed cytogenetics data on chromatin conformation, and the arrangement and mutual positioning of chromosome territories in interphase nuclei are still widely missing in plants. In this study, level of chromatin condensation in interphase nuclei of rice (Oryza sativa) and the distribution of chromosome territories (CTs) were analyzed. Super-resolution, stimulated emission depletion (STED) microscopy showed different levels of chromatin condensation in leaf and root interphase nuclei. 3D immuno-FISH experiments with painting probes specific to chromosomes 9 and 2 were conducted to investigate their spatial distribution in root and leaf nuclei. Six different configurations of chromosome territories, including their complete association, weak association, and complete separation, were observed in root meristematic nuclei, and four configurations were observed in leaf nuclei. The volume of CTs and frequency of their association varied between the tissue types. The frequency of association of CTs specific to chromosome 9, containing NOR region, is also affected by the activity of the 45S rDNA locus. Our data suggested that the arrangement of chromosomes in the nucleus is connected with the position and the size of the nucleolus.

Accession Number: WOS:001242916700001

PubMed ID: 38863533

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Doležalová, Alžběta	GYQ-9212-2022	

ISSN: 1664-462X

Record 217 of 274

Title: Feasibility of perturbative generation of bound states from resonances or virtual states

Author(s): Yang, CJ (Yang, C. -J.)

Source: PHYSICAL REVIEW C **Volume:** 109 **Issue:** 5 **Article Number:** 054003 **DOI:** 10.1103/PhysRevC.109.054003 **Published Date:** 2024 MAY 24 **Supplement:** DOI:

Abstract: I investigate whether it is possible to generate bound states from resonances or virtual states through first -order perturbation theory. Using contact -type potentials as those appeared in pionless effective field theory, I show that it is possible to obtain negative -energy states by sandwiching a next -to -leading order interaction with the leading -order (LO) wave functions, under the presence of LO resonances or virtual states. However, at least under the framework of time -independent Schr ödinger equation and Hermitian Hamiltonian, there is an inability to create bound states with structure similar to those formed by the nonperturbative treatments.

Accession Number: WOS:001237292700001

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ISSN: 2469-9985

eISSN: 2469-9993

Record 218 of 274

Title: Classification with costly features in hierarchical deep sets

Author(s): Janisch, J (Janisch, Jaromir); Pevny, T (Pevny, Tomas); Lisy, V (Lisy, Viliam)

Source: MACHINE LEARNING **Volume:** 113 **Issue:** 7 **Pages:** 4487-4522 **DOI:** 10.1007/s10994-024-06565-4 **Early Access Date:** MAY 2024 **Published Date:** 2024 JUL

Abstract: Classification with costly features (CwCF) is a classification problem that includes the cost of features in the optimization criteria. Individually for each sample, its features are sequentially acquired to maximize accuracy while minimizing the acquired features' cost. However, existing approaches can only process data that can be expressed as vectors of fixed length. In real life, the data often possesses rich and complex structure, which can be more precisely described with formats such as XML or JSON. The data is hierarchical and often contains nested lists of objects. In this work, we extend an existing deep reinforcement learning-based algorithm with hierarchical deep sets and hierarchical softmax, so that it can directly process this data. The extended method has greater control over which features it can acquire and, in experiments with seven datasets, we show that this leads to superior performance. To showcase the real usage of the new method, we apply it to a real-life problem of classifying malicious web domains, using an online service.

Accession Number: WOS:001229224200001

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Pevny, Tomas	E-1984-2018	
Janisch, Jaromir		0000-0002-4165-6503

ISSN: 0885-6125
eISSN: 1573-0565

Record 219 of 274

Title: Optimizing properties of translocation-enhancing transmembrane proteins

Author(s): Bartos, L (Bartos, Ladislav); Drabinová, M (Drabinova, Martina); Vácha, R (Vacha, Robert)

Source: BIOPHYSICAL JOURNAL **Volume:** 123 **Issue:** 10 **Pages:** 1240-1252 **DOI:** 10.1016/j.bpj.2024.04.009 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 21

Abstract: Cell membranes act as semi-permeable barriers, often restricting the entry of large or hydrophilic molecules. Nonetheless, certain amphiphilic molecules, such as antimicrobial and cell-penetrating peptides, can cross these barriers. In this study, we demonstrate that specific properties of transmembrane proteins/peptides can enhance membrane permeation of amphiphilic peptides. Using coarse-grained molecular dynamics with free-energy calculations, we identify key translocation-enhancing attributes of transmembrane proteins/peptides: a continuous hydrophilic patch, charged residues preferably in the membrane center, and aromatic hydrophobic residues. By employing both coarse-grained and atomistic simulations, complemented by experimental validation, we show that these properties not only enhance peptide translocation but also speed up lipid flip-flop. The enhanced flip-flop reinforces the idea that proteins such as scramblases and insertases not only share structural features but also operate through identical biophysical mechanisms enhancing the insertion and translocation of amphiphilic molecules. Our insights offer guidelines for the designing of translocation-enhancing proteins/peptides that could be used in medical and biotechnological applications. SIGNIFICANCE Cells are enveloped by a selectively permeable cytoplasmic membrane. Certain peptides can spontaneously penetrate this protective barrier, serving as potential drug carriers or therapeutic agents. In this study, we demonstrate that the translocation of peptides across membrane into cell can be enhanced with the passive assistance of transmembrane proteins. We investigate various properties of these transmembrane proteins that enhance the translocation and we establish guidelines for designing such translocation enhancers. We show that these enhancers also facilitate lipid scrambling, which suggests more general effect on amphiphilic molecules. Therefore, proteins facilitating the insertion of amphiphilic molecules into the membrane's hydrophobic core, such as translocation enhancers, insertases, translocases, and scramblases, might share a common biophysical mechanism.

Accession Number: WOS:001300570200001

PubMed ID: 38615194

ISSN: 0006-3495

eISSN: 1542-0086

Record 220 of 274

Title: A statistical framework for a new Kavya-Manoharan Bilal distribution using ranked set sampling and simple random sampling

Author(s): Shafiq, A (Shafiq, Anum); Sindhu, TN (Sindhu, Tabassum Naz); Riaz, MB (Riaz, Muhammad Bilal); Hassan, MKH (Hassan, Marwa K. H.); Abushal, TA (Abushal, Tahani A.)

Source: HELIYON **Volume:** 10 **Issue:** 9 **Article Number:** e30762 **DOI:** 10.1016/j.heliyon.2024.e30762 **Published Date:** 2024 MAY 15

Abstract: In survival and stochastic lifespan modeling, numerous families of distributions are sometimes considered unnatural, unjustifiable theoretically, and occasionally superfluous. Here, a novel parsimonious survival model is developed using the Bilal distribution (BD) and the KavyaManoharan (KM) parsimonious transformation family. In addition to other analytical properties, the forms of probability density function (PDF) and behavior of the distributions ' hazard rates are analyzed. The insights are theoretical as well as practical. Theoretically, we offer explicit equations for the single and product moments of order statistics from Kavya-Manoharan Bilal Distribution. Practically, maximum likelihood (ML) technique, which is based on simple random sampling (SRS) and ranked set sampling

(RSS) sample schemes, is employed to estimate the parameters. Numerical simulations are used as the primary methodology to compare the various sampling techniques.

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PubMed ID: 38765132

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Riaz, Muhammad	ABA-9824-2021	
Shafiq, Anum	F-9967-2018	
Sindhu, Tabassum	AAR-5257-2020	0000-0001-9433-4981

eISSN: 2405-8440

Record 221 of 274

Title: Properties of multiple Lewis acid sites in alkali metal-exchanged chabazites probed by CO adsorption

Author(s): Halamek, J (Halamek, Jakub); Bulánek, R (Bulanek, Roman); Rubes, M (Rubes, Miroslav); Bludsky, O (Bludsky, Ota)

Source: MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 374 **Article Number:** 113152 **DOI:** 10.1016/j.micromeso.2024.113152 **Early Access Date:** MAY 2024 **Published Date:** 2024 JUN 15

Abstract: Carbon monoxide adsorption on alkali -metal exchanged chabazites (M- CHA , where M = Li, Na, K) was investigated across various Si/Al ratios. The study reveals significant insights into the adsorption behavior, including the persistence of cationic preferences with decreasing Si/Al ratios and the existence of multiple -center interactions involving alkali -metal cations and CO. Results show that for high -silica MCHA zeolites, CO adsorption is effectively described by single and dual adsorption site models, with cation preferences varying by type. In low -silica zeolites, cation positions are primarily influenced by the aluminum distribution and Coulombic interactions. However, the propensity for single -site cation positions (Si/Al ->infinity) is preserved to a certain degree. The most noticeable example is the small difference between SIII ' occupancies (cations in 8 -membered ring windows) in Na- CHA -2 and K- CHA -2 (0.80 vs. 0.85) that strongly influences the rate of diffusion of CO in the MCHA -2 samples. While FT-IR spectra of high -silica zeolites can be accurately described using cation site stabilities, interaction energies, and CO stretching frequencies, predicting spectra of low -silica chabazites requires a statistical approach and/or molecular dynamics simulations at the DFT level. The findings demonstrate that the dynamical behavior of adsorbates changes dramatically between different alkali metal -exchanged chabazites, highlighting the complex nature of CO adsorption at multiple Lewis acid sites.

Accession Number: WOS:001237195200001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rubes, Miroslav	GPF-5266-2022	

ISSN: 1387-1811

eISSN: 1873-3093

Record 222 of 274

Title: Mechanisms of Ligand Hyperfine Coupling in Transition-Metal Complexes: σ and π Transmission Pathways

Author(s): Novotny, J (Novotny, Jan); Munzarová, M (Munzarova, Marketa); Marek, R (Marek, Radek)

Source: INORGANIC CHEMISTRY **Volume:** 63 **Issue:** 19 **Pages:** 8580-8592 **DOI:** 10.1021/acs.inorgchem.3c04425 **Early Access Date:** MAY 2024 **Published Date:** 2024 MAY 1

Abstract: Theoretical interpretation of hyperfine interactions was pioneered in the 1950s-1960s by the seminal works of McConnell, Karplus, and others for organic radicals and by Watson and Freeman for transition-metal (TM) complexes. In this work, we investigate a series of octahedral Ru(III) complexes with aromatic ligands to understand the mechanism of transmission of the spin density from the d-orbital of the metal to the s-orbitals of the ligand atoms. Spin densities and spin populations underlying ligand hyperfine couplings are analyzed in terms of pi-conjugative or sigma-hyperconjugative delocalization vs spin polarization based on symmetry considerations and restricted open-shell vs unrestricted wave function analysis. The transmission of spin density is shown to be most efficient in the case of symmetry-allowed pi-conjugative delocalization, but when the pi-conjugation is partially or fully symmetry-forbidden, it can be surpassed by sigma-hyperconjugative delocalization. Despite a lower spin population of the ligand in sigma-hyperconjugative transmission, the hyperfine couplings can be larger because of the direct involvement of the ligand s-orbitals in this delocalization pathway. We demonstrate a quantitative correlation between the hyperfine couplings of aromatic ligand atoms and the characteristics of the metal-ligand bond modulated by the trans substituent, a hyperfine trans effect.

Accession Number: WOS:001227850700001

PubMed ID: 38690843

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Novotny, Jan	D-7676-2012	
Marek, Radek	D-6929-2012	

ISSN: 0020-1669

eISSN: 1520-510X

Record 223 of 274

Title: Ternary recombination of excited Ar⁺(<mml:mmultiscripts>P1/2<mml:none/><mml:mprescripts/><mml:none/>2</mml:mmultiscripts>) ions, established experimental results reinterpreted with a new extended model

Author(s): Nongni, FT (Nongni, F. T.); Kalus, R (Kalus, R.); Benhenni, M (Benhenni, M.); Gadéa, FX (Gadea, F. X.); Yousfi, M (Yousfi, M.)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 160 **Issue:** 16 **Article Number:** 161101 **DOI:** 10.1063/5.0202524 **Published Date:** 2024 APR 28

Abstract: For many years, the recombination of excited ions of argon, Ar+(P1/22), has been assumed negligible under ambient conditions as compared to the recombination of ground-state ions, Ar+(P3/22). This opinion was confronted with detailed experimental results that seem to clearly support it. Here, we propose a new interpretation in light of our recent calculations, which shows that the recombination efficiency is comparable for both fine-structure states. Noteworthily, in our model leading to a picture consistent with the experiment, residual dimer ions emerge from Ar+(P1/22) due to non-adiabatic dynamics effects and interplay in measured data.

Accession Number: WOS:001206881000015

PubMed ID: 38647297

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kalus, René	O-6552-2017	

ISSN: 0021-9606

eISSN: 1089-7690

Record 224 of 274

Title: Comment on "Numerical study with OpenFOAM on heat conduction problems in heterogeneous media" by K. Zhang, C.-A. Wang, J.-Y. Tan, International Journal of Heat and Mass Transfer, Vol. 124 (2018) 1156-1162

Author(s): Bohacek, J (Bohacek, J.); Mraz, K (Mraz, K.); Hvozda, J (Hvozda, J.); Lang, F (Lang, F.); Karimi-Sibaki, E (Karimi-Sibaki, E.); Vakhrushev, A (Vakhrushev, A.); Kharicha, A (Kharicha, A.)

Source: INTERNATIONAL JOURNAL OF HEAT AND MASS TRANSFER **Volume:** 227 **Article Number:** 125603 **DOI:** 10.1016/j.ijheatmasstransfer.2024.125603 **Early Access Date:** APR 2024 **Published Date:** 2024 AUG 1

Abstract: In the paper "Numerical study with OpenFOAM on heat conduction problems in heterogeneous media" by K. Zhang, C. -A. Wang, J. -Y. Tan, International Journal of Heat and Mass Transfer, Vol. 124 (2018) 1156-1162 the authors modify laplacianFoam from open -source CFD package OpenFOAM (R) to solve heat conduction problems in heterogeneous media by changing the diffusion coefficient from a constant value to a scalar field. Their paper clearly demonstrates a fundamental, overlooked, and common mistake in rearranging the heat conduction equation, which cannot be replaced with the temperature diffusion equation. In this comment, we provide clear evidence through mathematical derivations and numerical examples calculated in OpenFOAM (R).

Accession Number: WOS:001232526800001

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ISSN: 0017-9310

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Record 225 of 274

Title: A new reactive Mo-S-C force field to explore structure and properties of MoS 2-C 2D materials and films

Author(s): Ponomarev, I (Ponomarev, Ilia); Polcar, T (Polcar, Tomas)

Source: COMPUTATIONAL MATERIALS SCIENCE **Volume:** 241 **Article Number:** 113034 **DOI:** 10.1016/j.commatsci.2024.113034 **Early Access Date:** APR 2024 **Published Date:** 2024 MAY 25

Abstract: We employed a Monte -Carlo optimization scheme to successfully create a novel ReaxFF parameter set tailored for the exploration of the structures and energetics of Mo-S-C materials. This force field underwent rigorous testing against Density Functional Theory (DFT) data and exhibited its efficacy in modeling a broad spectrum of structures, ranging from composite heterolayer 2D structures to fully amorphous coatings. Subsequently, we applied this force field to get insights into the structural formation of amorphous MoS 2 -C films. Our simulations yielded promising results, revealing, in agreement with the experimental findings, preferential formation of Mo-S and C -C bonds along with rapid phase segregation.

Accession Number: WOS:001218422100001

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Ponomarev, Ilia		0000-0002-3321-6671

ISSN: 0927-0256
eISSN: 1879-0801

Record 226 of 274

Title: Ancient hybridization and repetitive element proliferation in the evolutionary history of the monocot genus Amomum (Zingiberaceae)

Author(s): Hlavatá, K (Hlavata, Kristyna); Záveská, E (Zaveska, Eliska); Leong-Skornicková, J (Leong-Skornickova, Jana); Pouch, M (Pouch, Milan); Poulsen, AD (Poulsen, Axel Dalberg); Sída, O (Sida, Otakar); Khadka, B (Khadka, Bijay); Mandáková, T (Mandakova, Terezie); Fér, T (Fer, Tomas)

Source: FRONTIERS IN PLANT SCIENCE **Volume:** 15 **Article Number:** 1324358 **DOI:** 10.3389/fpls.2024.1324358 **Published Date:** 2024 APR 19

Abstract: Genome size variation is a crucial aspect of plant evolution, influenced by a complex interplay of factors. Repetitive elements, which are fundamental components of genomic architecture, often play a role in genome expansion by selectively amplifying specific repeat motifs. This study focuses on Amomum, a genus in the ginger family (Zingiberaceae), known for its 4.4-fold variation in genome size. Using a robust methodology involving PhyloNet reconstruction, RepeatExplorer clustering, and repeat similarity-based phylogenetic network construction, we investigated the repeatome composition, analyzed repeat dynamics, and identified potential hybridization events within the genus. Our analysis confirmed the presence of four major infrageneric clades (A-D) within Amomum, with clades A-C exclusively comprising diploid species (2n = 48) and clade D encompassing both diploid and tetraploid species (2n = 48 and 96). We observed an increase in the repeat content within the genus, ranging from 84% to 89%, compared to outgroup species with 75% of the repeatome. The SIRE lineage of the Ty1-Copia repeat superfamily was prevalent in most analyzed ingroup genomes. We identified significant difference in repeatome structure between the basal Amomum clades (A, B, C) and the most diverged clade D. Our investigation revealed evidence of ancient hybridization events within Amomum, coinciding with a substantial proliferation of multiple repeat groups. This finding supports the hypothesis that ancient hybridization is a driving force in the genomic evolution of Amomum. Furthermore, we contextualize our findings within the broader context of genome size variations and repeatome dynamics observed across major monocot lineages. This study enhances our understanding of evolutionary processes within monocots by highlighting the crucial roles of repetitive elements in shaping genome size and suggesting the mechanisms that drive these changes.

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PubMed ID: 38708400

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Fér, Tomáš	A-9991-2008	

ISSN: 1664-462X

Record 227 of 274

Title: Influence of proline and hydroxyproline as antimicrobial and anticancer peptide components on the silver(I) ion activity: structural and biological evaluation with a new theoretical and experimental SAR approach

Author(s): Kuzderová, G (Kuzderova, Gabriela); Sovová, S (Sovova, Simona); Rendosová, M (Rendosova, Michaela); Gyepes, R (Gyepes, Robert); Sabolová, D (Sabolova, Danica); Kozárová, I (Kozarova, Ivona); Balázová, L (Balazova, Ludmila); Vilková, M (Vilkova, Maria); Kello, M (Kello, Martin); Liska, A (Liska, Alan); Vargová, Z (Vargova, Zuzana)

Source: DALTON TRANSACTIONS **Volume:** 53 **Issue:** 26 **DOI:** 10.1039/d4dt00389f **Early Access Date:** APR 2024 **Published Date:** 2024 JUL 2

Abstract: Silver(I) complexes with proline and hydroxyproline were synthesized and structurally characterized and crystal structure analysis shows that the formulas of the compounds are {[Ag-2(Pro)(2)(NO3)]NO3}(n) (AgPro) (Pro = L-proline) and {[Ag-2(Hyp)(2)(NO3)]NO3}(n) (AgHyp) (Hyp = trans-4-hydroxy-L-proline). Both complexes crystallize in the monoclinic lattice with space group P2(1) with a carboxylate bidentate-bridging coordination mode of the organic ligands Pro and Hyp (with NH2+ and COO- groups in zwitterionic form). Both complexes have a distorted seesaw (C-2v) geometry around one silver(I) ion with tau(4) values of 58% (AgPro) and 51% (AgHyp). Moreover, the results of spectral and thermal analyses correlate with the structural ones. H-1 and C-13 NMR spectra confirm the complexes species' presence in the DMSO biological testing medium and their stability in the time range of the bioassays. In addition, molar conductivity measurements indicate complexes' behaviour like 1 : 1 electrolytes. Both complexes showed higher or the same antibacterial activity against Bacillus cereus, Pseudomonas aeruginosa and Staphylococcus aureus as AgNO3 (MIC = 0.063 mM) and higher than silver(I) sulfadiazine (AgSD) (MIC > 0.5 mM) against Pseudomonas aeruginosa. In addition, complex AgPro exerted a strong cytotoxic effect against the tested MDA-MB-231 and Jurkat cancer cell lines (IC50 values equal to 3.7 and 3.0 mu M, respectively) compared with AgNO3 (IC50 = 6.1 (5.7) mu M) and even significantly higher selectivity than cisplatin (cisPt) against MDA-MB-231 cancer cell lines (SI = 3.05 (AgPro); 1.16 (cisPt), SI - selectivity index). The binding constants and the number of binding sites (n) of AgPro and AgHyp complexes with bovine serum albumin (BSA) were determined at four different temperatures, and the zeta potential of BSA in the presence of silver(I) complexes was also measured. The in ovo method shows the safety of the topical and intravenous application of AgPro and AgHyp. Moreover, the complexes' bioavailability was verified by lipophilicity evaluation from the experimental and theoretical points of view.

Accession Number: WOS:001207922300001

PubMed ID: 38661536

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Liska, Alan	O-4810-2014	
Vilková, Mária	A-5151-2017	
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Gyepes, Robert	F-5192-2014	0000-0002-2908-0425
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ISSN: 1477-9226

eISSN: 1477-9234

Record 228 of 274

Title: Atomic-scale stick-slip through a point defect

Author(s): Gnecco, E (Gnecco, Enrico); Nicolini, P (Nicolini, Paolo)

Source: PHYSICAL REVIEW B **Volume:** 109 **Issue:** 13 **Article Number:** 134103 **DOI:** 10.1103/PhysRevB.109.134103 **Published Date:** 2024 APR 10

Abstract: We have derived a series of analytical formulas describing the motion of a nanotip elastically driven across a Gaussian potential well of depth U-1 and half width sigma. The tip gets pinned if the impact parameter y(0) is below a well-defined threshold value. Together with U-1 and sigma , this value determines the pinning force. The scenario is slightly modified by superimposing a periodic potential with amplitude U-0 in the background, provided that U-0 << U-1. The formulas presented here can be applied to estimate the pinning energy and the linear extension of the perturbation created by a point defect such as an atomic vacancy on a crystal surface from atomic-scale friction force measurements performed by scanning probe microscopy.

Accession Number: WOS:001247348100003

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Nicolini, Paolo	D-9151-2012	0000-0003-1324-7566

ISSN: 2469-9950

eISSN: 2469-9969

Record 229 of 274

Title: Impact of swaps on Mossbauer characteristics of Ni₂MnSn: an experimental and quantum-mechanical study

Author(s): Friák, M (Friak, Martin); Schneeweiss, O (Schneeweiss, Oldrich); Kamarád, J (Kamarad, Jiri); Kastil, J (Kastil, Jiri); Miroshkina, ON (Miroshkina, Olga N.); Gruner, ME (Gruner, Markus E.)

Source: JOURNAL OF MATERIALS SCIENCE **Volume:** 59 **Issue:** 13 **Pages:** 5595-5606 **DOI:** 10.1007/s10853-024-09515-6 **Published Date:** 2024 APR

Abstract: We report on a combined experimental and theoretical study of stoichiometric Heusler-structure Ni2MnSn. Our detected Mossbauer spectrum of Sn atoms can be fitted as a combination of four components. As only a single component is expected in the defect-free Ni2MnSn, we have performed quantum-mechanical calculations of Ni2MnSn with selected point defects, in particular, all three fundamental types of swaps (Mn-Ni, Mn-Sn and Ni-Sn). Our phonon and elasticity calculations indicate that the swaps result in (i) magnitudes of local magnetic moments of Sn atoms within four ranges of values and (ii) mean square displacements of Sn atoms falling within four intervals of values. Further, we used calculations of phonons and elastic properties to assess mechanical, dynamical and thermodynamic stability of swap-containing states. Our results indicate that a majority of the studied swaps is reducing the stability of Ni2MnSn and need to be stabilized by the surrounding matrix.

Accession Number: WOS:001265093200008

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ISSN: 0022-2461

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Record 230 of 274

Title: On the Possible Effect of Phytic Acid (Myo-Inositol Hexaphosphoric Acid, IP6) on Cytochromes P450 and Systems of Xenobiotic Metabolism in Different Hepatic Models

Author(s): Frybortova, V (Frybortova, Veronika); Satka, S (Satka, Stefan); Jourova, L (Jourova, Lenka); Zapletalova, I (Zapletalova, Iveta); Srejber, M (Srejber, Martin); Briolotti, P (Briolotti, Philippe); Daujat-Chavanieu, M (Daujat-Chavanieu, Martine); Gerbal-Chaloin, S (Gerbal-Chaloin, Sabine); Anzenbacher, P (Anzenbacher, Pavel); Otyepka, M (Otyepka, Michal); Anzenbacherova, E (Anzenbacherova, Eva)

Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES **Volume:** 25 **Issue:** 7 **Article Number:** 3610 **DOI:** 10.3390/ijms25073610 **Published Date:** 2024 APR

Abstract: As compounds of natural origin enter human body, it is necessary to investigate their possible interactions with the metabolism of drugs and xenobiotics in general, namely with the cytochrome P450 (CYP) system. Phytic acid (myo-inositol hexaphosphoric acid, IP6) is mainly present in plants but is also

an endogenous compound present in mammalian cells and tissues. It has been shown to exhibit protective effect in many pathological conditions. For this paper, its interaction with CYPs was studied using human liver microsomes, primary human hepatocytes, the HepG2 cell line, and molecular docking. Docking experiments and absorption spectra demonstrated the weak ability of IP6 to interact in the heme active site of CYP1A. Molecular docking suggested that IP6 preferentially binds to the protein surface, whereas binding to the active site of CYP1A2 was found to be less probable. Subsequently, we investigated the ability of IP6 to modulate the metabolism of xenobiotics for both the mRNA expression and enzymatic activity of CYP1A enzymes. Our findings revealed that IP6 can slightly modulate the mRNA levels and enzyme activity of CYP1A. However, thanks to the relatively weak interactions of IP6 with CYPs, the chances of the mechanisms of clinically important drug-drug interactions involving IP6 are low.

Accession Number: WOS:001201042000001

PubMed ID: 38612422

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ISSN: 1661-6596

eISSN: 1422-0067

Record 231 of 274

Title: Two-dimensional Janus transition-metal carbide for flexible anode through surface engineering

Author(s): Fu, ZH (Fu, Zhongheng); Wang, N (Wang, Ning); Shi, CX (Shi, Chongxing); Legut, D (Legut, Dominik); Chen, X (Chen, Xiang); Zhang, RF (Zhang, Ruifeng); Zhang, DW (Zhang, Dawei)

Source: APPLIED SURFACE SCIENCE **Volume:** 659 **Article Number:** 159944 **DOI:** 10.1016/j.apsusc.2024.159944 **Early Access Date:** MAR 2024 **Published Date:** 2024 JUN 30

Abstract: Two-dimensional transition metal carbides (MXenes) have received tremendous attention because of their great promise in flexible energy storage. Although surface engineering plays an important role in regulating the properties of MXenes with the development of synthesis technology, an atomistic design of surface diversity for desired functionalities is generally limited by purely unified surface termination. Herein, the Janus MXenes consisting of different surface terminations are proposed for flexible anodes through first-principles calculations. Taking Ti2CTT' (T, T' = O, F, or OH) as an illustration of Janus MXenes, critical strains, ideal strengths, Li-ion diffusion barriers, equilibrium voltages, and theoretical capacities are determined and used as descriptors to evaluate the properties of flexible anodes. These Janus MXenes exhibit high critical strains and ideal strengths, indicating their mechanical flexibility. The strain-independent Li-ion diffusion barrier of Ti2COF suggests its fast Li-ion transport even suffering from mechanical deformation, endowing its application potential in flexible anodes. These results establish a theoretical framework for the comprehensive evaluation of flexible anode materials, providing a theoretical scheme for designing flexible anode materials.

Accession Number: WOS:001223410700001

Author Identifiers:

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Zhang, Dawei	R-8835-2019	
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ISSN: 0169-4332
eISSN: 1873-5584

Record 232 of 274

Title: On the parallel solution of hydro-mechanical problems with fracture networks and contact conditions

Author(s): Stebel, J (Stebel, Jan); Kruzík, J (Kruzik, Jakub); Horák, D (Horak, David); Brezina, J (Brezina, Jan); Béres, M (Beres, Michal)

Source: COMPUTERS & STRUCTURES **Volume:** 298 **Article Number:** 107339 **DOI:** 10.1016/j.compstruc.2024.107339 **Early Access Date:** MAR 2024 **Published Date:** 2024 JUL 15

Abstract: The paper presents a numerical method for simulating flow and mechanics in fractured rock. The governing equations that couple the effects in the rock mass and in the fractures are obtained using the discrete fracturematrix approach. The fracture flow is driven by the cubic law, and the contact conditions prevent fractures from self -penetration. A stable finite element discretization is proposed for the displacement -pressure -flux formulation. The resulting nonlinear algebraic system of equations and inequalities is decoupled using a robust iterative splitting into the linearized flow subproblem, and the quadratic programming problem for the mechanical part. The non -penetration conditions are solved by means of dualization and an optimal quadratic programming algorithm. The capability of the numerical scheme is demonstrated on a benchmark problem for tunnel excavation with hundreds of fractures in 3D. The paper's novelty consists in a combination of three crucial ingredients: (i) application of discrete fracture -matrix approach to poroelasticity, (ii) robust iterative splitting of resulting nonlinear algebraic system working for real -world 3D problems, and (iii) efficient solution of its mechanical quadratic programming part with a large number of fractures in mutual contact by means of own solvers implemented into an in-house software library.

Accession Number: WOS:001217402600001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 0045-7949
eISSN: 1879-2243

Record 233 of 274

Title: Distribution and Functional Analysis of Isocitrate Dehydrogenases across Kinetoplastids

Author(s): Chmelová, L (Chmelova, Lubomira); Záhonová, K (Zahonova, Kristina); Albanaz, ATS (Albanaz, Amanda T. S.); Hrebenyk, L (Hrebenyk, Liudmyla); Horváth, A (Horvath, Anton); Yurchenko, V (Yurchenko, Vyacheslav); Skodová-Sveráková, I (Skodova-Sverakova, Ingrid)

Source: GENOME BIOLOGY AND EVOLUTION **Volume:** 16 **Issue:** 3 **Article Number:** evae042 **DOI:** 10.1093/gbe/evae042 **Early Access Date:** MAR 2024 **Published Date:** 2024 MAR 2

Abstract: Isocitrate dehydrogenase is an enzyme converting isocitrate to alpha-ketoglutarate in the canonical tricarboxylic acid (TCA) cycle. There are three different types of isocitrate dehydrogenase documented in eukaryotes. Our study points out the complex evolutionary history of isocitrate dehydrogenases across kinetoplastids, where the common ancestor of Trypanosomatidae and Bodonidae was equipped with two isoforms of the isocitrate dehydrogenase enzyme: the NADP(+)-dependent isocitrate dehydrogenase 1 with possibly dual localization in the cytosol and mitochondrion and NADP(+)-dependent mitochondrial isocitrate dehydrogenase 2. In the extant trypanosomatids, isocitrate dehydrogenase 1 is present only in a few species suggesting that it was lost upon separation of Trypanosoma spp. and replaced by the mainly NADP+-dependent cytosolic isocitrate dehydrogenase 3 of

bacterial origin in all the derived lineages. In this study, we experimentally demonstrate that the omnipresent isocitrate dehydrogenase 2 has a dual localization in both mitochondrion and cytosol in at least four species that possess only this isoform. The apparent lack of the NAD(+)-dependent isocitrate dehydrogenase activity in trypanosomatid mitochondrion provides further support to the existence of the noncanonical TCA cycle across trypanosomatids and the bidirectional activity of isocitrate dehydrogenase 3 when operating with NADP(+) cofactor instead of NAD(+). This observation can be extended to all 17 species analyzed in this study, except for Leishmania mexicana, which showed only low isocitrate dehydrogenase activity in the cytosol. The variability in isocitrate oxidation capacity among species may reflect the distinct metabolic strategies and needs for reduced cofactors in particular environments.

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PubMed ID: 38447055

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Záhonová, Kristína	AAT-9188-2020	
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Zahonova, Kristina		0000-0002-5766-0267
Yurchenko, Vyacheslav	E-4532-2013	0000-0003-4765-3263

ISSN: 1759-6653

Record 234 of 274

Title: Mechanistic insights into interactions between ionizable lipid nanodroplets and biomembranes

Author(s): Cechová, P (Cechova, Petra); Paloncyová, M (Paloncyova, Marketa); Srejber, M (Srejber, Martin); Otyepka, M (Otyepka, Michal)

Source: JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS **DOI:** 10.1080/07391102.2024.2329307 **Early Access Date:** MAR 2024 **Published Date:** 2024 MAR 9

Abstract: Delivery of RNA into cells using lipid nanoparticles (LNPs) has been a significant breakthrough in RNA-based medicine, with clinical applicability expanded through the use of ionizable lipids (ILs). These unique lipids can alter their charge state in response to pH changes, which is crucial for pH-triggered endosomal escape and effective lipid-mediated RNA delivery. In this study, we conducted a comprehensive set of molecular dynamics (MD) simulations to investigate interactions between IL-containing lipid nanodroplets (LNDs) and cell membrane models. Using an atomistic resolution model, we investigated the merging process of LNDs with cell membrane models under neutral conditions relevant to an intercellular environment and acidic pH conditions found in late endosomes. Our observations revealed that at neutral pH, LNDs merged with lipid membranes while preserving the bilayer structure. Under acidic conditions, the LNDs remained attached to the bilayer without fusing into the membranes. Importantly, the presence of ILs did not disrupt the original biomembrane structure during the simulation period. The MD simulations provided valuable atomistic insights into the mechanism of interaction between IL-containing nanodroplets and biomembranes, which could aid the rational design of ILs to develop more efficient LNPs for RNA therapies.

Accession Number: WOS:001185421500001

PubMed ID: 38487842

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 0739-1102

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Record 235 of 274

Title: Hot subdwarf wind models with accurate abundances II. Helium-dominated merger products CD-46 8926 and CD-51 11879

Author(s): Krticka, J (Krticka, J.); Krtickova, I (Krtickova, I.); Janík, J (Janik, J.); Németh, P (Nemeth, P.); Kubát, J (Kubat, J.); Vuckovic, M (Vuckovic, M.)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 683 **Article Number:** A80 **DOI:** 10.1051/0004-6361/202347978 **Published Date:** 2024 MAR 8

Abstract: Context. Helium-dominated subdwarfs are core helium burning stars stripped of their envelope. The nuclear evolution of these stars alters surface abundances. Modified abundances impact the strength of the stellar wind. Aims. We aim to understand the influence of modified surface abundances on the strength of the stellar wind in the helium-dominated subdwarfs CD-46 8926 and CD-51 11879. A modified wind strength could resolve the problem with the X-ray emission of these stars, as the expected X-ray luminosity of both stars is significantly higher than the upper limit determined from observations. Methods. We used our own optical spectroscopy combined with archival ultraviolet spectroscopy and photometry to derive basic parameters and surface abundances of selected subdwarfs. The resulting parameterst served as input for the METUJE stellar wind code, which predicts the wind structure of these stars. We compared the derived wind parameters with the predictions derived for solar abundances. Results. The optical analysis showed that both subdwarfs have effective temperatures in excess of 60 kK and a strong overabundance of carbon in the case of CD-46 8926 and nitrogen in the case of CD-51 11879. We interpret the abundance patterns as being a result of enrichment by the products of nuclear reactions. The modified abundances reduce the wind mass-loss rate by tens of percent. The reduction improves the predicted wind line profiles in comparison to observations. The change in helium abundance does not have a strong effect on the wind parameters. As a result of a lower estimated bolometric luminosity and mass-loss rate and a larger distance, the expected X-ray luminosities become lower and agree with observational upper limits. Conclusions. The nucleosynthesis does not significantly alter the strength of the wind of hot subdwarfs, but the inclusion of proper stellar parameters improves the agreement with observational wind characteristics. Our analysis indicates that subdwarfs overabundant in helium are typically able to launch wind. This conclusion is supported by data gathered for thousands of subdwarfs from the literature, which shows that subdwarfs overabundant in helium avoid the region in the Kiel diagram where the winds are predicted to be absent. This can be interpreted in terms of the gravitational settling of helium, which is suppressed by the winds.

Accession Number: WOS:001181364400009

Author Identifiers:

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Nemeth, Peter	E-4515-2016	
Kubat, Jiri	G-9032-2014	0000-0003-4269-8278

ISSN: 0004-6361

eISSN: 1432-0746

Record 236 of 274

Title: Modeling and analysis of hybrid-blood nanofluid flow in stenotic artery

Author(s): Sarwar, L (Sarwar, Lubna); Hussain, A (Hussain, Azad); Riaz, MB (Riaz, Muhammad Bilal); Akbar, S (Akbar, Sobia)

Source: SCIENTIFIC REPORTS **Volume:** 14 **Issue:** 1 **Article Number:** 5409 **DOI:** 10.1038/s41598-024-55621-5 **Published Date:** 2024 MAR 5

Abstract: Current communication deals with the flow impact of blood inside cosine shape stenotic artery. The under consideration blood flow is treated as Newtonian fluid and flow is assumed to be two dimensional. The governing equation are modelled and solved by adopting similarity transformation under the stenosis assumptions. The important quantities like Prandtl number, flow parameter, blood flow rate and skin friction are attained to analyze the blood flow phenomena in stenosis. The variations of different parameters have been shown graphically. It is of interest to note that velocity increases due to change in flow parameter gamma and temperature of blood decreases by increasing nanoparticles volume fraction and Prandtl number. In the area of medicine, the most interesting nanotechnology approach is the nanoparticles applications in chemotherapy. This study provides further motivation to include more convincing consequences in the present model to represent the blood rheology.

Accession Number: WOS:001180457200005

PubMed ID: 38443416

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Riaz, Muhammad	ABA-9824-2021	

ISSN: 2045-2322

Record 237 of 274

Title: Point defects in Dirac semimetal BeN₄ monolayer and their interaction with gas molecules

Author(s): Erdem, I (Erdem, Isa); Bilican, F (Bilican, Fuat); Kart, HH (Kart, Hasan Huseyin); Kart, SO (Kart, Sevgi Ozdemir); Ersan, F (Ersan, Fatih)

Source: VACUUM **Volume:** 222 **Article Number:** 113095 **DOI:** 10.1016/j.vacuum.2024.113095 **Early Access Date:** MAR 2024 **Published Date:** 2024 APR

Abstract: Point defects in materials may occur during the fabrication process of monolayer materials, or these defects can be created via electron beam irradiation to the perfect crystals. Recently, a triclinic phase of beryllium tetranitride BeN4 was synthesized from elements at similar to 85 GPa pressure and can become a monolayer under ambient conditions. In this study, we have introduced various point defects into the BeN4 monolayer such as Be or N mono vacancy (Be-vac, N-vac), Be-N divacancy (Be-N-vac), antisite defect of Be-N atomic positions and Stone-Wales (SW) defect, and investigated electronic and magnetic changes in the material. It is found that with the Be vacancy, the Dirac cone of the BeN4 monolayer disappears and the Be-vac. monolayer shows semi-metallic properties with overlapping valence and conduction bands. N vacancy induces local magnetic moment (0.797 mu B) to the structure, and the N-vac monolayer has a direct band gap value of 0.172 eV. While the Be-N divacancy turns the structure to metal, the antisite-defected BeN4 monolayer turns into a non-magnetic semiconductor with a band gap value of 0.256 eV. Furthermore, we have introduced bare and defected BeN4 monolayers with CO, CO2, H-2, H2O and O-2 gas molecules and found that these molecules give rise to crucial effects on the electronic and magnetic properties of the materials. While the considered molecules are physisorbed on the bare BeN4 monolayer, the H2O molecule dissociated to OH and H on the N-vac structure, and O-2 molecule strongly binds on N-vac and antisite BeN4 monolayers. Furthermore, we have reported that the antisite BeN4 monolayer may be a good candidate material for hydrogen storage devices with an adsorption energy of 0.355 eV of the H-2 molecule. We believe that our theoretical findings will be beneficial for further experimental and theoretical studies on BeN4 structure.

Accession Number: WOS:001207878600001

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ISSN: 0042-207X

eISSN: 1879-2715

Record 238 of 274

Title: On Recursion Operators for Full-Fledged Nonlocal Symmetries of the Reduced Quasi-classical Self-dual Yang-Mills Equation

Author(s): Jahnová, J (Jahnova, Jirina); Vojcák, P (Vojcak, Petr)

Source: ANNALES HENRI POINCARE **Volume:** 25 **Issue:** 10 **Pages:** 4633-4669 **DOI:** 10.1007/s00023-024-01425-2 **Early Access Date:** MAR 2024 **Published Date:** 2024 OCT

Abstract: We introduce the idea of constructing recursion operators for full-fledged nonlocal symmetries and apply it to the reduced quasi-classical self-dual Yang-Mills equation. It turns out that the discovered recursion operators can be interpreted as infinite-dimensional matrices of differential functions which act on the generating vector functions of the nonlocal symmetries simply by matrix multiplication. To the best of our knowledge, there are no other examples of such recursion operators in the literature so far, so our approach is completely innovative. Further, we investigate the algebraic properties of the discovered operators and discuss the R\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$ ${\mathbb {R}}$$\end{document}-algebra structure on the set of all recursion operators for full-fledged nonlocal symmetries of the equation in question. Finally, we illustrate the action of the obtained recursion operators on particularly chosen full-fledged symmetries and emphasize their advantages compared to the action of traditionally used recursion operators for shadows.

Accession Number: WOS:001172954900001

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Jahnova, Jirina		0009-0007-9127-2886

ISSN: 1424-0637

eISSN: 1424-0661

Record 239 of 274

Title: A Computational Characterization of CH₄@C₆₀

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

Source: INORGANICS **Volume:** 12 **Issue:** 3 **Article Number:** 64 **DOI:** 10.3390/inorganics12030064 **Published Date:** 2024 MAR

Abstract: The recently synthetically prepared endohedral CH4@C-60 was characterized here using calculations-namely its structure, energetics, thermodynamics, and vibrational spectrum. The calculations were carried out with DFT (density-functional theory) methods, namely by the DFT M06-2X functional

and MP2, as well as B2PLYPD advanced correlated, treatments with the standard 6-31++G** and 6-311++G** basis sets, corrected for the basis set superposition error evaluated using the approximative Boys-Bernardi counterpoise method. The symmetry of the endohedral obtained in the geometry optimizations was tetrahedral T. The energetics of CH4 encapsulation into C-60 was attractive (i.e., with a negative encapsulation-energy term), producing a substantial energy gain of -13.94 kcal/mol at the most advanced computational level, B2PLYPD/6-311++G**. The encapsulation equilibrium constants for CH4@C-60 were somewhat higher than previously found with the CO@C-60 system. For example at 500 K, the encapsulation equilibrium constant for CH4@C-60 had a value one order of magnitude larger than for CO@C-60. The encapsulation thermodynamic characteristics suggest that high-pressure and high-temperature synthesis could in principle also be possible for CH4@C-60.

Accession Number: WOS:001193460900001

Author Identifiers:

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Uhlik, Filip	G-7395-2012	

eISSN: 2304-6740

Record 240 of 274

Title: Exploring analytical solutions and modulation instability for the nonlinear fractional Gilson-Pickering equation

Author(s): Rahman, RU (Rahman, Riaz Ur); Riaz, MB (Riaz, Muhammad Bilal); Martinovic, J (Martinovic, Jan); Tunc, O (Tunc, Osman)

Source: RESULTS IN PHYSICS **Volume:** 57 **Article Number:** 107385 **DOI:** 10.1016/j.rinp.2024.107385 **Early Access Date:** FEB 2024 **Published Date:** 2024 FEB

Abstract: The primary goal of this research is to explore the complex dynamics of wave propagation as described by the nonlinear fractional Gilson-Pickering equation (fGPE), a pivotal model in plasma physics and crystal lattice theory. Two alternative fractional derivatives, termed fi and M -truncated, are employed in the analysis. The new auxiliary equation method (NAEM) is applied to create diverse explicit solutions for surface waves in the given equation. This study includes a comparative evaluation of these solutions using different types of fractional derivatives. The derived solutions of the nonlinear fGPE, which include unique forms like dark, bright, and periodic solitary waves, are visually represented through 3D and 2D graphs. These visualizations highlight the shapes and behaviors of the solutions, indicating significant implications for industry and innovation. The proposed method's ability to provide analytical solutions demonstrates its effectiveness and reliability in analyzing nonlinear models across various scientific and technical domains. A comprehensive sensitivity analysis is conducted on the dynamical system of the f GPE. Additionally, modulation instability analysis is used to assess the model's stability, confirming its robustness. This analysis verifies the stability and accuracy of all derived solutions.

Accession Number: WOS:001179230400001

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ISSN: 2211-3797

Record 241 of 274

Title: Highly resolved genome assembly and comparative transcriptome profiling reveal genes related to developmental stages of tapeworm Ligula intestinalis

Author(s): Nazarizadeh, M (Nazarizadeh, Masoud); Nováková, M (Novakova, Milena); Drábková, M (Drabkova, Marie); Catchen, J (Catchen, Julian); Olson, PD (Olson, Peter D.); Stefka, J (Stefka, Jan)

Source: PROCEEDINGS OF THE ROYAL SOCIETY B-BIOLOGICAL SCIENCES **Volume:** 291 **Issue:** 2015 **Article Number:** 20232563 **DOI:** 10.1098/rspb.2023.2563 **Published Date:** 2024 JAN 31

Abstract: Ligula intestinalis (Cestoda: Diphyllobothriidae) is an emerging model organism for studies on parasite population biology and host-parasite interactions. However, a well-resolved genome and catalogue of its gene content has not been previously developed. Here, we present the first genome assembly of L. intestinalis, based on Oxford Nanopore Technologies, Illumina and Omni-C sequencing methodologies. We use transcriptome profiling to compare plerocercoid larvae and adult worms and identify differentially expressed genes (DEGs) associated with these life stages. The genome assembly is 775.3 mega (M)bp in size, with scaffold N50 value of 118 Mbp and encodes 27 256 predicted protein-coding sequences. Over 60% of the genome consists of repetitive sequences. Synteny analyses showed that the 10 largest scaffolds representing 75% of the genome display high correspondence to full chromosomes of cyclophyllidean tapeworms. Mapping RNA-seq data to the new reference genome, we identified 3922 differentially expressed genes in adults compared with plerocercoids. Gene ontology analyses revealed over-represented genes involved in reproductive development of the adult stage (e.g. sperm production) and significantly enriched DEGs associated with immune evasion of plerocercoids in their fish host. This study provides the first insights into the molecular biology of L. intestinalis and provides the most highly contiguous assembly to date of a diphyllobothriid tapeworm useful for population and comparative genomic investigations of parasitic flatworms.

Accession Number: WOS:001153940600006

PubMed ID: 38290545

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ISSN: 0962-8452

eISSN: 1471-2954

Record 242 of 274

Title: Dynamics of collisions and uptake of alcohol molecules with hydrated nitric acid clusters

Author(s): Fárníková, K (Farnikova, Karolina); Pluharová, E (Pluharova, Eva); Pysanenko, A (Pysanenko, Andrij); Fárník, M (Farnik, Michal); Yan, YH (Yan, Yihui); Lengyel, J (Lengyel, Jozef)

Source: FARADAY DISCUSSIONS **Volume:** 251 **Issue:** 0 **Pages:** 296-312 **DOI:** 10.1039/d3fd00160a **Early Access Date:** JAN 2024 **Published Date:** 2024 AUG 27

Abstract: We investigate the collisions of different alcohol molecules with hydrated nitric acid clusters using a molecular beam experiment and molecular dynamics simulations. The uptake cross sections sigma p for the molecules evaluated from the experiment are in excellent agreement with the simulations. This suggests that (i) the nontrivial assumptions implemented in the evaluation procedure of the experimental data are valid, and (ii) the simulations describe correctly the major processes in the molecule-cluster collisions. We observe that sigma p decreases with the increasing alkyl chain length of the alcohol, and also with the branching of the molecules that have the same mass but different

structures. These systematic trends can be rationalized based on the accessibility of the hydrophilic OH group, which decreases with the increasing chain length and steric hindrance. The observed trends and their interpretation differ significantly from the simple model of hard-sphere collisions. The obtained data shall be beneficial not only for the fundamental understanding of the molecule-cluster collisions, but also in the modelling of atmospheric new-particle formation and aerosol growth.
The uptake cross sections in collisions of different alcohol molecules with hydrated nitric acid clusters are measured using a molecular beam experiment. Complementary molecular dynamics simulations elucidate the processes.

Accession Number: WOS:001224873700001

PubMed ID: 38758164

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ISSN: 1359-6640

eISSN: 1364-5498

Record 243 of 274

Title: The Impact of ortho-substituents on Bonding in Silver(I) and Halogen(I) Complexes of 2-Mono- and 2,6-Disubstituted Pyridines: An In-Depth Experimental and Theoretical Study

Author(s): Kumar, P (Kumar, Parveen); Rautiainen, JM (Rautiainen, J. Mikko); Novotny, J (Novotny, Jan); Ward, JS (Ward, Jas S.); Marek, R (Marek, Radek); Rissanen, K (Rissanen, Kari); Puttreddy, R (Puttreddy, Rakesh)

Source: CHEMISTRY-A EUROPEAN JOURNAL **Volume:** 30 **Issue:** 13 **DOI:** 10.1002/chem.202303643 **Early Access Date:** JAN 2024 **Published Date:** 2024 MAR 1

Abstract: The coordination nature of 2-mono- and 2,6-disubstituted pyridines with electron-withdrawing halogen and electron-donating methyl groups for [N-X-N](+) (X=I, Br) complexations have been studied using N-15 NMR, X-ray crystallography, and Density Functional Theory (DFT) calculations. The N-15 NMR chemical shifts reveal iodine(I) and bromine(I) prefer to form complexes with 2-substituted pyridines and only 2,6-dimethylpyridine. The crystalline halogen(I) complexes of 2-substituted pyridines were characterized by using X-ray diffraction analysis, but 2,6-dihalopyridines were unable to form stable crystalline halogen(I) complexes due to the lower nucleophilicity of the pyridinic nitrogen. In contrast, the halogen(I) complexes of 2,6-dimethylpyridine, which has a more basic nitrogen, are characterized by X-crystallography, which complements the N-15 NMR studies. DFT calculations reveal that the bond energies for iodine(I) complexes vary between -291 and -351 kJ mol(-1) and for bromine between -370 and -427 kJ mol(-1). The bond energies of halogen(I) complexes of 2-halopyridines with more nucleophilic nitrogen are 66-76 kJ mol(-1) larger than those of analogous 2,6-dihalopyridines with less nucleophilic nitrogen. The experimental and DFT results show that the electronic influence of ortho-halogen substituents on pyridinic nitrogen leads to a completely different preference for the coordination bonding of halogen(I) ions, providing new insights into bonding in halogen(I) chemistry.

Accession Number: WOS:001143279900001

PubMed ID: 38055221

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ISSN: 0947-6539

eISSN: 1521-3765

Record 244 of 274

Title: Conformations and hydration of halopropionic acids studied by molecular dynamics and Raman optical activity

Author(s): Beresová, M (Beresova, Marie); Bufka, J (Bufka, Jiri); Safarík, M (Safarik, Martin); Bour, P (Bour, Petr); Sebestík, J (Sebestik, Jaroslav)

Source: SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY **Volume:** 309 **Article Number:** 123852 **DOI:** 10.1016/j.saa.2024.123852 **Early Access Date:** JAN 2024 **Published Date:** 2024 MAR 15

Abstract: Chiral 2-halopropionic acids and their derivatives were synthesized and their properties studied computationally using Raman and Raman optical activity (ROA) spectroscopy. For neat acids present as liquids small amount of water led to significant changes in the spectra, resulting even to flipping of some ROA band signs. We find this interesting for the role water plays in interpretation of vibrational optical activity spectra of biomolecules. Analysis of the results shows that when the water is present, it can change ROA band signs due to the changes in acidobasic equilibrium. Corresponding esters without acidic hydrogens do not exhibit such effects.

Accession Number: WOS:001164123600001

PubMed ID: 38217987

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Bufka, Jiri	LEM-0450-2024	
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ISSN: 1386-1425

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Record 245 of 274

Title: Stimulated radiative association of sodium and chlorine atoms and their ions in a coupled channel treatment

Author(s): Zamecniková, MSN (Zamecnikova, Martina Simsova Nee); Gustafsson, M (Gustafsson, Magnus); Nyman, G (Nyman, Gunnar); Soldán, P (Soldan, Pavel)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 26 **Issue:** 4 **Pages:** 3342-3349 **DOI:** 10.1039/d3cp05602c **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN 24

Abstract: In an extension of previous work (Simsova et al., Phys. Chem. Chem. Phys., 2022, 24, 25250), we study stimulated radiative association of sodium chloride (NaCl) in an environment with a black body radiation. Colliding neutral (Na and Cl) and ionic (Na+ and Cl-) fragments are considered. The coupling

between the diabatic ionic and neutral channels is accounted for. The cross sections are computed and resolved on the vibrational states of the formed NaCl molecule for detailed analysis. The thermal rate coefficients for neutral colliding fragments at kinetic temperatures, T, from 1 K to 5300 K are computed for use in astrochemical modelling. The total rate coefficient is affected by more than one order of magnitude by stimulated emission from a blackbody radiator of temperature Tb = 50 000 K. The effect from stimulated emission is largest for the lowest kinetic temperatures, where Tb of a few thousand kelvins has a significant effect. The rate coefficient for the colliding ionic fragments is calculated from 80 K to 3615 K. The blackbody radiation has little effect on this process.
Formation of NaCl by radiative association is studied by non-adiabatic dynamics at background temperatures ranging up to 50 000 K.

Accession Number: WOS:001139341600001

PubMed ID: 38198198

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ISSN: 1463-9076

eISSN: 1463-9084

Record 246 of 274

Title: On the origin of the electronic and magnetic circular dichroism of naphthyl C-glycosides: Anomeric configuration

Author(s): Choutka, J (Choutka, Jan); Parkan, K (Parkan, Kamil); Pohl, R (Pohl, Radek); Kaminsky, J (Kaminsky, Jakub)

Source: CARBOHYDRATE RESEARCH **Volume:** 535 **Article Number:** 109021 **DOI:** 10.1016/j.carres.2023.109021 **Early Access Date:** JAN 2024 **Published Date:** 2024 JAN

Abstract: Aryl C-glycosides, in which the glycosidic bond is changed to a carbon-carbon bond, are an important family of biologically-active compounds. They often serve as secondary metabolites or exhibit antibiotic and cytostatic activities. Their stability to hydrolysis has made them attractive targets for new drugs. Their conformational behavior often strongly influences the resulting function. Their detailed structural and conformational description is thus highly desirable. This work studies the structure of three different naphthyl C-glycosides using UV-vis absorption as well as electronic and magnetic circular dichroism. It also describes their conformational preferences using a combination of molecular dynamics and DFT calculations. The reliability of these preferences has been verified by simulations of spectral properties and a comparison with their measured spectra. In particular, ECD spectroscopy has been shown to distinguish easily between alpha- and beta-pseudoanomers of aryl C-glycosides. Computer simulations and spectral decomposition have revealed how the resulting ECD patterns of the naphthyl glycosides studied are influenced by different conformer populations. In conclusion, reliable ECD patterns cannot be calculated by separating the naphthyl rotation from other conformational motions. MCD patterns have been similar for all the naphthyl C-glycosides studied. No clear diagnostic features have been found for either the pseudoanomeric configuration or the preferred hydroxymethyl rotamer. Nevertheless, the work has demonstrated the potential of MCD for the study of aryl glycosides interacting with proteins.

Accession Number: WOS:001154687800001

PubMed ID: 38171193

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ISSN: 0008-6215

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Record 247 of 274

Title: Breaking DPA-Protected Kyber via the Pair-Pointwise Multiplication

Author(s): Bock, EA (Bock, Estuardo Alpirez); Banegas, G (Banegas, Gustavo); Brzuska, C (Brzuska, Chris); Chmielewski, L (Chmielewski, Lukasz); Puniamurthy, K (Puniamurthy, Kirthivaasan); Sorf, M (Sorf, Milan)

Edited by: Popper C; Batina L

Source: APPLIED CRYPTOGRAPHY AND NETWORK SECURITY, ACNS 2024, PT II **Book Series:** Lecture Notes in Computer Science **Volume:** 14584 **Pages:** 101-130 **DOI:** 10.1007/978-3-031-54773-7_5 **Published Date:** 2024

Abstract: We introduce a novel template attack for secret key recovery in Kyber, leveraging side-channel information from polynomial multiplication during decapsulation. Conceptually, our attack exploits that Kyber's incomplete number-theoretic transform (NTT) causes each secret coefficient to be used multiple times, unlike when performing a complete NTT.
Our attack is a single trace known ciphertext attack that avoids machine-learning techniques and instead relies on correlation-matching only. Additionally, our template generation method is very simple and easy to replicate, and we describe different attack strategies, varying on the number of templates required. Moreover, our attack applies to both masked implementations as well as designs with multiplication shuffling.
We demonstrate its effectiveness by targeting a masked implementation from the mkm4 repository. We initially perform simulations in the noisy Hamming-Weight model and achieve high success rates with just 13 316 templates while tolerating noise values up to sigma = 0.3. In a practical setup, we measure power consumption and notice that our attack falls short of expectations. However, we introduce an extension inspired by known online template attacks, enabling us to recover 128 coefficient pairs from a single polynomial multiplication. Our results provide evidence that the incomplete NTT, which is used in Kyber-768 and similar schemes, introduces an additional side-channel weakness worth further exploration.

Accession Number: WOS:001206023700005

Conference Title: 22nd International Conference on Applied Cryptography and Network Security (ACNS)

Conference Date: MAR 05-08, 2024

Conference Location: Abu Dhabi, U ARAB EMIRATES

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ISSN: 0302-9743

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ISBN: 978-3-031-54772-0; 978-3-031-54773-7

Record 248 of 274

Title: Investigating Portability in Chapel for Tree-Based Optimization on GPU-Powered Clusters

Author(s): Carneiro, T (Carneiro, Tiago); Kayraklioglu, E (Kayraklioglu, Engin); Helbecque, G (Helbecque, Guillaume); Melab, N (Melab, Nouredine)

Edited by: Carretero J; Shende S; Garcia-Blas J; Brandic I; Olcoz K; Schreiber M

Source: EURO-PAR 2024: PARALLEL PROCESSING, PT III, EURO-PAR 2024 **Book Series:** Lecture Notes in Computer Science **Volume:** 14803 **Pages:** 386-399 **DOI:** 10.1007/978-3-031-69583-4_27 **Published Date:** 2024

Abstract: The Top500 list features supercomputers powered by accelerators from different vendors. This variety brings, along with the heterogeneity challenge, both the code and performance portability challenges. In this context, Chapel's native GPU support comes as a solution for code portability between different vendors. In this paper, we investigate the viability of using the Chapel high-productivity language as a tool to achieve both code and performance portability in large-scale tree-based search. As a case study, we implemented a distributed backtracking for solving permutation combinatorial problems. Extensive experiments conducted on big N-Queens problem instances, using up to 512 NVIDIA GPUs and 1024 AMD GPUs on Top500 supercomputers, reveal that it is possible to scale on the two different systems using the same tree-based search written in Chapel. This trade-off results in a performance decrease of less than 10% for the biggest problem instances.

Accession Number: WOS:001308371400027

Conference Title: 30th European Conference on Parallel and Distributed Processing (Euro-Par)

Conference Date: AUG 26-30, 2024

Conference Location: Madrid, SPAIN

Conference Sponsors: Univ Carlos III, Dept Comp Sci & Engn

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ISBN: 978-3-031-69582-7; 978-3-031-69583-4

Record 249 of 274

Title: QUANTUM-COMPUTING STUDY OF THE ELECTRONIC STRUCTURE OF CRYSTALS: THE CASE STUDY OF SI

Author(s): Duriska, M (Duriska, Michal); Miháliková, I (Mihalikova, Ivana); Friák, M (Friak, Martin)

Book Group Author(s): Tanger Ltd

Source: 15TH INTERNATIONAL CONFERENCE ON NANOMATERIALS-RESEARCH & APPLICATION, NANOCON 2023 **Book Series:** NANOCON Conference Proceedings **Pages:** 40-45 **DOI:** 10.37904/nanocon.2023.4774 **Published Date:** 2024

Abstract: Quantum computing is newly emerging information-processing technology which is foreseen to be exponentially faster than classical supercomputers. Current quantum processors are nevertheless very limited in their availability and performance and many important software tools for them do not exist yet. Therefore, various systems are studied by simulating the run of quantum computers. Building upon our previous experience with quantum computing of small molecular systems (see I. Mihalikova et al., Molecules 27 (2022) 597, and I. Mihalikova et al., Nanomaterials 2022, 12, 243), we have recently focused on computing electronic structure of periodic crystalline materials. Being inspired by the work of Cerasoli et al. (Phys. Chem. Chem. Phys., 2020, 22, 21816), we have used hybrid variational quantum eigensolver (VQE) algorithm, which combined classical and quantum information processing. Employing tight-binding type of crystal description, we present our results for crystalline diamond-structure silicon. In particular, we focus on the states along the lowest occupied band within the

electronic structure of Si and compare the results with values obtained by classical means. While we demonstrate an excellence agreement between classical and quantum-computed results in most of our calculations, we further critically check the sensitivity of our results with respect to computational set-up in our quantum-computing study. A few results were obtained also using quantum processors provided by the IBM.

Accession Number: WOS:001234125400006

Conference Title: 15th International Conference on Nanomaterials-Research & Application (NANOCON)

Conference Date: OCT 18-20, 2023

Conference Location: Brno, CZECH REPUBLIC

ISSN: 2694-930X

ISBN: 978-80-88365-15-0

Record 250 of 274

Title: QUANTUM-MECHANICAL STUDY OF INTERNAL STRUCTURAL TRANSFORMATIONS IN Pb-SUPERSATURATED Pb-Sn ALLOYS

Author(s): Friák, M (Friak, Martin); Cípek, P (Cipek, Petr); Pavlu, J (Pavlu, Jana); Roupcová, P (Roupcova, Pavla); Miháliková, I (Mihalikova, Ivana); Msallamová, S (Msallamova, Sarka); Michalcová, A (Michalcova, Alena)

Book Group Author(s): Tanger Ltd

Source: 15TH INTERNATIONAL CONFERENCE ON NANOMATERIALS-RESEARCH & APPLICATION, NANOCON 2023 **Book Series:** NANOCON Conference Proceedings **Pages:** 15-21 **DOI:** 10.37904/nanocon.2023.4749 **Published Date:** 2024

Abstract: Motivated by a decades-long controversy related to the crystal structure of Pb-supersaturated solid solutions of Pb in Sn, we have performed a quantum-mechanical study of these materials. Focusing on both body-centred-tetragonal beta-Sn and simple-hexagonal gamma-Sn structures, we have computed properties of two alloys with the chemical composition Pb5Sn11, i.e. 31.25 at. % Pb, which is close to the composition of the experimentally found alloy (30 at. % Pb). The 16-atom computational supercells were designed as multiples of the elemental beta- and gamma-Sn unit cells, where the Pb atoms were distributed according to the special quasi-random structure (SQS) concept. Full structural relaxations of both beta- and gamma-phase-based alloys resulted in very significant re-arrangements into structures which do not exhibit any apparent structural features typical for the original alloys, and are, therefore, difficult to classify. The formation energies of the beta- and gamma-phase-originating equilibrium phases are 50 meV/atom and 53 meV/atom, respectively. Therefore, they are not stable with respect to the decomposition into the elemental lead and tin. Moreover, our calculations of elastic constants of both phases revealed that they are close to mechanical instability. Our results indicate that the studied Pb-supersaturated Pb-Sn solid solutions may be prone to structural instability, transformations into different phases and decomposition. Our findings may contribute into the identification of the reason why the subsequent experimental studies did not reproduce the initial published data.

Accession Number: WOS:001234125400002

Conference Title: 15th International Conference on Nanomaterials-Research & Application (NANOCON)

Conference Date: OCT 18-20, 2023

Conference Location: Brno, CZECH REPUBLIC

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pavlu, Jana	E-3482-2012	

ISSN: 2694-930X

ISBN: 978-80-88365-15-0

Record 251 of 274

Title: Windower: Feature Extraction for Real-Time DDoS Detection Using Machine Learning

Author(s): Goldschmidt, P (Goldschmidt, Patrik); Kucera, J (Kucera, Jan)

Edited by: Hong JWK; Seok SJ; Nomura Y; Wang YC; Choi BY; Kim MS; Riggio R; Tsai MH; DosSantos CRP

Source: PROCEEDINGS OF 2024 IEEE/IFIP NETWORK OPERATIONS AND MANAGEMENT SYMPOSIUM, NOMS 2024 **Book Series:** IEEE IFIP Network Operations and Management Symposium **DOI:** 10.1109/NOMS59830.2024.10575699 **Published Date:** 2024

Abstract: Distributed Denial of Service (DDoS) attacks are an ever-increasing type of security incident on modern computer networks. To tackle the issue, we propose Windower, a feature-extraction method for real-time network-based intrusion (particularly DDoS) detection. Our stream data mining module employs a sliding window principle to compute statistical information directly from network packets.

Furthermore, we summarize several such windows and compute inter-window statistics to increase detection reliability. Summarized statistics are then fed into an ML-based attack discriminator. If an attack is recognized, we drop the consequent attacking source's traffic using simple ACL rules. The experimental results evaluated on several datasets indicate the ability to reliably detect an ongoing attack within the first six seconds of its start and mitigate 99% of flood and 92% of slow attacks while maintaining false positives below 1%. In contrast to state-of-the-art, our approach provides greater flexibility by achieving high detection performance and low resources as flow-based systems while offering prompt attack detection known from packet-based solutions. Windower thus brings an appealing trade-off between attack detection performance, detection delay, and computing resources suitable for real-world deployments.

Accession Number: WOS:001270140300170

Conference Title: IEEE/IFIP Network Operations and Management Symposium (NOMS)

Conference Date: MAY 06-10, 2024

Conference Location: Seoul, SOUTH KOREA

Conference Sponsors: IEEE

ISSN: 1542-1201

ISBN: 979-8-3503-2793-9; 979-8-3503-2794-6

Record 252 of 274

Title: Data Alignment and Duration Modelling in VITS

Author(s): Hanzlícek, Z (Hanzlicek, Zdenek)

Edited by: Noth E; Horak A; Sojka P

Source: TEXT, SPEECH, AND DIALOGUE, TSD 2024, PT II **Book Series:** Lecture Notes in Artificial Intelligence **Volume:** 15049 **Pages:** 118-129 **DOI:** 10.1007/978-3-031-70566-3_11 **Published Date:** 2024

Abstract: The paper analyses data alignment and duration modelling in the modern end-to-end speech synthesis model VITS (Variational Inference with adversarial learning for end-to-end Text-to-Speech). The standard version of VITS utilizes the MAS (Monotonic Alignment Search) procedure to align input text/phones and corresponding speech during the training procedure; the alignment is also used to obtain phoneme durations for the stochastic duration predictor training. This study analyzes the resulting MAS alignment and compares it with a reference alignment obtained by an LSTM-based phonetic segmentation system. We also examine the performance of VITS when the reference phonetic segmentation replaces the default MAS alignment. The comparison shows that while the original VITS is still slightly preferred in terms of quality, it provides a less interpretative data alignment. The duration modelling is more transparent in the modified version, allowing better duration control and modifications. The analysis has been carried out on two Czech voices.

Accession Number: WOS:001307848400011

Conference Title: 27th International Conference on Text, Speech, and Dialogue (TSD)

Conference Date: SEP 09-13, 2024

Conference Location: Brno, CZECH REPUBLIC

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Hanzlíček, Zdeněk	GYJ-0173-2022	

ISSN: 2945-9133

eISSN: 1611-3349

ISBN: 978-3-031-70565-6; 978-3-031-70566-3

Record 253 of 274

Title: FAIR Sharing of Data in Autotuning Research (Vision Paper)

Author(s): Hozzová, J (Hozzova, Jana); Torring, JO (Torring, Jacob O.); van Werkhoven, B (van Werkhoven, Ben); Strelák, D (Strelak, David); Vuduc, R (Vuduc, Richard)

Book Group Author(s): ASSOC COMPUTING MACHINERY

Source: COMPANION OF THE 15TH ACM/SPEC INTERNATIONAL CONFERENCE ON PERFORMANCE ENGINEERING, ICPE COMPANION 2024 **Pages:** 21-27 **DOI:** 10.1145/3629527.3651429 **Published Date:** 2024

Abstract: Autotuning is an automated process that selects the best computer program implementation from a set of candidates to improve performance, such as execution time, when run under new circumstances, such as new hardware. The process of autotuning generates a large amount of performance data with multiple potential use cases, including reproducing results, comparing included methods, and understanding the impact of individual tuning parameters. We propose the adoption of FAIR Principles, which stands for Findable, Accessible, Interoperable, and Reusable, to organize the guidelines for data sharing in autotuning research. The guidelines aim to lessen the burden of sharing data and provide a comprehensive checklist of recommendations for shared data. We illustrate three examples that could greatly benefit from shared autotuning data to advance the research without time- and resource-demanding data collection.
To facilitate data sharing, we have taken a community-driven approach to define a common format for the data using a JSON schema and provide scripts for their collection.
The proposed comprehensive guide for collecting and sharing performance data in autotuning research can promote further advances in the field and encourage research collaboration.

Accession Number: WOS:001227617500004

Conference Title: 15th ACM/SPEC International Conference on Performance Engineering (ICPE)

Conference Date: MAY 07-11, 2024

Conference Location: Imperial Coll London, London, ENGLAND

Conference Sponsors: Assoc Comp Machinery, SPEC Res, ACM SIGMETRICS, ACM Special Interest Grp Software Engn

Conference Host: Imperial Coll London

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ISBN: 979-8-4007-0445-1

Record 254 of 274

Title: A Compiler for Weak Decomposable Negation Normal Form

Author(s): Illner, P (Illner, Petr); Kucera, P (Kucera, Petr)

Edited by: Wooldridge M; Dy J; Natarajan S

Source: THIRTY-EIGHTH AAAI CONFERENCE ON ARTIFICIAL INTELLIGENCE, VOL 38 NO 9 **Book Series:** AAAI Conference on Artificial Intelligence **Pages:** 10562-10570 **Published Date:** 2024

Abstract: This paper integrates weak decomposable negation normal form (wDNNF) circuits, introduced by Akshay et al. in 2018, into the knowledge compilation map. This circuit type generalises decomposable negation normal form (DNNF) circuits in such a way that they allow a restricted form of sharing variables among the inputs of a conjunction node. We show that wDNNF circuits have the same properties as DNNF circuits regarding the queries and transformations presented in the knowledge compilation map, whilst being strictly more succinct than DNNF circuits (that is, they can represent Boolean functions compactly). We also present and evaluate a knowledge compiler, called Bella, for converting CNF formulae into wDNNF circuits. Our experiments demonstrate that wDNNF circuits are suitable for configuration instances.

Accession Number: WOS:001241512400129

Conference Title: 38th AAAI Conference on Artificial Intelligence (AAAI) / 36th Conference on Innovative Applications of Artificial Intelligence / 14th Symposium on Educational Advances in Artificial Intelligence

Conference Date: FEB 20-27, 2024

Conference Location: Vancouver, CANADA

Conference Sponsors: Assoc Advancement Artificial Intelligence

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 2159-5399

eISSN: 2374-3468

Record 255 of 274

Title: Acceleration of Ultrasound Neurostimulation Using Mixed-Precision Arithmetic

Author(s): Jaros, J (Jaros, Jiri); Duchon, R (Duchon, Radek)

Book Group Author(s): Assoc Computing Machinery

Source: PROCEEDINGS OF THE 33RD INTERNATIONAL SYMPOSIUM ON HIGH-PERFORMANCE PARALLEL AND DISTRIBUTED COMPUTING, HPDC 2024 **DOI:** 10.1145/3625549.3658823 **Published Date:** 2024

Abstract: Ultrasound neurostimulation, a technique that modulates the brain's electrical activity, has emerged as a significant secondary treatment option for cases resistant to pharmacological interventions. The therapy is achievable through the application of a three-dimensional steerable ultrasound, directed by patient-specific stimulation plans. These plans are meticulously crafted through full-wave ultrasound propagation simulations. Nonetheless, the computational intensity required for calculating these plans poses a significant challenge, often reaching the memory capacities of contemporary graphics processing units (GPUs). By representing material properties and k-space operators more efficiently, we achieved up to 22% reduction in GPU memory usage, while accelerating calculations by 8.5% on an Nvidia Volta V100. This optimization introduced an error that reduced focal pressure by 0.5% without any focus movement, values that are clinically acceptable.

Accession Number: WOS:001305813000035

Conference Title: 33rd International Symposium on High-Performance Parallel and Distributed Computing (HPDC)

Conference Date: JUN 03-07, 2024

Conference Location: Pisa, ITALY

Conference Sponsors: ACM SIGARCH, E4 COMPUTER ENGN, VAST, CORNELIS NETWORKS, NEC Laboratories Amer

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Jaros, Jiri	H-2445-2016	

ISBN: 979-8-4007-0413-0

Record 256 of 274

Title: Deep-Learning Based Automatic Determination of Cardiac Planes in Survey MRI Data

Author(s): Jurca, J (Jurca, Jan); Harabis, V (Harabis, Vratislav); Jakubicek, R (Jakubicek, Roman); Holecek, T (Holecek, Tomas); Nemcekova, P (Nemcekova, Petra); Ourednicek, P (Ourednicek, Petr); Chmelik, J (Chmelik, Jiri)

Edited by: Badnjevic A; Pokvic LG

Source: MEDICON 2023 AND CMBEBIH 2023, VOL 1 **Book Series:** IFMBE Proceedings **Volume:** 93 **Pages:** 285-292 **DOI:** 10.1007/978-3-031-49062-0_31 **Published Date:** 2024

Abstract: Inference of the radiological planes of the heart in MRI is a crucial step for valid data acquisition to examine the structure and function of the human heart in detail. In this paper, we present a deep learning model for automatic inference of the radiological plane of the heart from 3D survey sequences. The proposed neural network is based on the V-Net [6] architecture that has been developed to perform inference on the radiological positions of the hearts. The network is designed to take a 3D image as input and generate a regressed heatmap of probable plane positions as output. The results show that the proposed method is feasible for automatic geometry planning. It has the potential to increase the efficiency of medical imaging. The presented networks show that they can locate cardiac landmarks even from data with anisotropic voxels. It can improve the accuracy and speed of diagnosis, allowing for faster and more effective treatment.

Accession Number: WOS:001261436400031

Conference Title: Mediterranean Conference on Medical and Biological Engineering and Computing (MEDICON) and International Conference on Medical and Biological Engineering (CMBEBIH)

Conference Date: SEP 14-16, 2023

Conference Location: Sarajevo, BOSNIA & HERCEG

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Harabis, Vratislav	D-5255-2014	
Jakubicek, Roman	D-3622-2018	
Chmelik, Jiri	H-9359-2017	0000-0001-9950-6279

ISSN: 1680-0737

ISBN: 978-3-031-49061-3; 978-3-031-49062-0

Record 257 of 274

Title: On 14-regular distance magic graphs

Author(s): Kovár, P (Kovar, Petr); Krbecek, M (Krbecek, Matej)

Source: ELECTRONIC JOURNAL OF GRAPH THEORY AND APPLICATIONS **Volume:** 12 **Issue:** 1 **Pages:** 35-41 **DOI:** 10.5614/ejgta.2024.12.1.4 **Published Date:** 2024

Abstract: Let G be a graph with n vertices. By N(v) we denote the set of all vertices adjacent to v. A bijection f : V(G) -> {1, 2, ... , n} is a distance magic labeling of G if there exists an integer k such that the sum of labels of all vertices adjacent to v is k for all vertices v in V(G). A graph which admits a distance magic labeling is a distance magic graph. In this paper, we completely characterize all orders for which a 14 -regular distance magic graph exists. Hereby we extended similar results on 2-, 4-, 6-, 8-, 10-, and 12 -regular distance magic graphs.

Accession Number: WOS:001217810700001

Author Identifiers:

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Kovar, Petr	E-9020-2012	0000-0002-7847-5060

ISSN: 2338-2287

Record 258 of 274

Title: Streamlining Neuroimaging - Snakemake's Role in Developing a Striatal Segmentation Pipeline

Author(s): Krajca, T (Krajca, Tomas); Marecek, S (Marecek, Stanislav); Sojka, P (Sojka, Petr); Dusek, P (Dusek, Petr); Krupicka, R (Krupicka, Radim)

Edited by: Costin HN; Magjarevic R; Petroiu GG

Source: ADVANCES IN DIGITAL HEALTH AND MEDICAL BIOENGINEERING, VOL 2, EHB-2023 **Book Series:** IFMBE Proceedings **Volume:** 110 **Pages:** 610-617 **DOI:** 10.1007/978-3-031-62520-6_68 **Published Date:** 2024

Abstract: The striatum, a component of the basal ganglia, has been extensively investigated in human and animal models due to its links to neurodegenerative diseases. One of the overarching goals of these studies is to identify biomarkers that can facilitate early detection during the prodromal or initial manifestation stages of these diseases. Various methods of diffusion magnetic resonance (dMRI) analysis are a promising avenue in human studies. A recent innovation provides a novel method of parceling the human striatum into distinct compartments with connectivity specific for the striosomes and matrix. This method involves numerous processing steps and requires significant computational resources. Integration of a scientific workflow is recommended to simplify deployment, ensure scalability and reliability, and facilitate the addition and parameterization of processes. This can potentially improve the efficiency of future research in this domain. In this study, we introduce a pipeline capable of segmenting striosome-like and matrix-like voxels in the human striatum using dMRI images, leveraging the scientific workflow tool, Snakemake.

Accession Number: WOS:001326809000068

Conference Title: 11th International Conference on E-Health and Bioengineering (EHB)

Conference Date: NOV 09-10, 2023

Conference Location: Univ Med & Pharmacy Iasi, Fac Med Bioengn, Bucharest, ROMANIA

Conference Sponsors: Int Soc Digital Health & Educat, Romanian Soc Med Bioengn, Inst Comp Sci Romanian Acad

Conference Host: Univ Med & Pharmacy Iasi, Fac Med Bioengn

Author Identifiers:

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Sojka, Petr	ABG-5688-2020	
Marecek, Stanislav	LXA-3151-2024	
Krupička, Radim	Q-1551-2019	
Dusek, Petr	F-9084-2017	
Marecek, Stanislav		0009-0004-0773-5373

ISSN: 1680-0737

ISBN: 978-3-031-62519-0; 978-3-031-62520-6

Record 259 of 274

Title: ON LINEAR MODELLING OF AXIAL VELOCITY DENSITY RATIO DEVELOPMENT IN COMPRESSOR BLADE CASCADES

Author(s): Kreuzová, T (Kreuzova, T.); Simurda, D (Simurda, D.); Safarík, P (Safarik, P.)

Edited by: Simurda D; Bodnar T

Source: TOPICAL PROBLEMS OF FLUID MECHANICS 2024 **Book Series:** Topical Problems of Fluid Mechanics **Pages:** 117-123 **DOI:** 10.14311/TPFM.2024.016 **Published Date:** 2024

Abstract: Flow field in transonic compressor blade cascade is examined by means of numerical simulations. Quasi-3D simulations with an influence of axial velocity density ratio (AVDR) are performed. Results of the simulations are compared to data available in literature. It is shown that modelling of AVDR as a linear function does not provide accurate predictions.

Accession Number: WOS:001242655400016

Conference Title: Conference on Topical Problems of Fluid Mechanics

Conference Date: FEB 21-23, 2024

Conference Location: Czech Acad Sci, Inst Thermomechan, Prague, CZECH REPUBLIC

Conference Sponsors: Czech Tech Univ, Fac Mech Engn, Dept Tech Math, Univ Toulon, Imath, ERCOFTAC, Czech Pilot Ctr

Conference Host: Czech Acad Sci, Inst Thermomechan

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ISSN: 2336-5781

ISBN: 978-80-87012-88-8

Record 260 of 274

Title: MINI Element for the Navier-Stokes System in 3D: Vectorized Codes and Superconvergence

Author(s): Kucera, R (Kucera, Radek); Arzt, V (Arzt, Vladimir); Koko, J (Koko, Jonas)

Source: INFORMATICA **Volume:** 35 **Issue:** 2 **Pages:** 341-361 **DOI:** 10.15388/24-INFOR543 **Published Date:** 2024

Abstract: A fast vectorized codes for assembly mixed finite element matrices for the generalized Navier-Stokes system in three space dimensions in the MATLAB language are proposed by the MINI element. Vectorization means that the loop over tetrahedra is avoided. Numerical experiments illustrate computational efficiency of the codes. An experimental superconvergence rate for the pressure component is established.

Accession Number: WOS:001230684700007

ISSN: 0868-4952

eISSN: 1822-8844

Record 261 of 274

Title: DiaPer: End-to-End Neural Diarization With Perceiver-Based Attractors

Author(s): Landini, F (Landini, Federico); Diez, M (Diez, Mireia); Stafylakis, T (Stafylakis, Themos); Burget, L (Burget, Lukas)

Source: IEEE-ACM TRANSACTIONS ON AUDIO SPEECH AND LANGUAGE PROCESSING **Volume:** 32 **Pages:** 3450-3465 **DOI:** 10.1109/TASLP.2024.3422818 **Published Date:** 2024

Abstract: Until recently, the field of speaker diarization was dominated by cascaded systems. Due to their limitations, mainly regarding overlapped speech and cumbersome pipelines, end-to-end models have gained great popularity lately. One of the most successful models is end-to-end neural diarization with encoder-decoder based attractors (EEND-EDA). In this work, we replace the EDA module with a Perceiver-based one and show its advantages over EEND-EDA; namely obtaining better performance on the largely studied Callhome dataset, finding the quantity of speakers in a conversation more accurately, and faster inference time. Furthermore, when exhaustively compared with other methods, our model, DiaPer, reaches remarkable performance with a very lightweight design. Besides, we perform comparisons with other works and a cascaded baseline across more than ten public wide-band datasets. Together with this publication, we release the code of DiaPer as well as models trained on public and free data.

Accession Number: WOS:001283673700005

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Landini, Federico	GWZ-8724-2022	
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ISSN: 2329-9290

eISSN: 2329-9304

Record 262 of 274

Title: Simulating Wind-Blown Nebulae from Single and Binary Massive Stars

Author(s): Mackey, J (Mackey, Jonathan)

Book Group Author(s): IOP

Source: 15TH INTERNATIONAL CONFERENCE ON NUMERICAL MODELING OF SPACE PLASMA FLOWS, ASTRONUM-2023 **Book Series:** Journal of Physics Conference Series **Volume:** 2742 **Article Number:** 012007 **DOI:** 10.1088/1742-6596/2742/1/012007 **Published Date:** 2024

Abstract: Winds from massive stars expand supersonically into their surroundings, creating dynamic and fascinating nebulae that can give us insight into physical processes in interstellar plasma, and into the evolutionary history of the stars. Around single stars, parsec-scale bubbles such as bow shocks and ring nebulae are formed, whereas in colliding-wind binary (CWB) systems the high wind density produces intense time- and space-dependent emission across the electromagnetic spectrum from radio to gamma-rays. This contribution summarizes some recent results from 3D MHD modelling of bow shocks around runaway stars such as zeta Oph, and of the wind-collision zone of the CWB systems WR140 and WR21a. A resolution study of 3D simulations of bow shocks shows that X-ray emission from the shocked wind is time-variable and that converged results can be obtained once the Kelvin-Helmholtz instability at the contact discontinuity is resolved. Simulations of the CWB system WR140 show that inverse-Compton cooling of the shocked plasma can trigger runaway cooling when the orbit is near periastron, producing strong compression and dynamical instabilities. This sharply reduces the hard-X-ray emission around periastron, in agreement with observations. Scaling tests of the simulation software pion are also presented for a model of the CWB system WR21a run on up to 8192 cores using the HPC system Karolina.

Accession Number: WOS:001214720200007

Conference Title: 15th International Conference on Numerical Modeling of Space Plasma Flows (ASTRONUM)

Conference Date: JUN 26-30, 2023

Conference Location: Pasadena, CA

Conference Sponsors: Univ Alabama Huntsville, Ctr Space Plasma & Aeron Res, French Alternat Energies, Maison Simulat, Atom Energy Commiss, Natl Ctr Sci Res, Univ Paris Saclay, Univ Versailles

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Author	Web of Science ResearcherID	ORCID Number
Mackey, Jonathan		0000-0002-5449-6131

ISSN: 1742-6588

eISSN: 1742-6596

Record 263 of 274

Title: Kernel Least Squares Transformations for Cross-Lingual Semantic Spaces

Author(s): Mistera, A (Mistera, Adam); Brychcín, T (Brychcin, Tomas)

Edited by: Horak A; Noth E; Sojka P

Source: TEXT, SPEECH, AND DIALOGUE, TSD 2024, PT I **Book Series:** Lecture Notes in Artificial Intelligence **Volume:** 15048 **Pages:** 227-238 **DOI:** 10.1007/978-3-031-70563-2_18 **Published Date:** 2024

Abstract: The rapid development in the field of natural language processing (NLP) and the increasing complexity of linguistic tasks demand the use of efficient and effective methods. Cross-lingual linear transformations between semantic spaces play a crucial role in this domain. However, compared to more advanced models such as transformers, linear transformations often fall short, especially in terms of accuracy. It is thus necessary to employ innovative approaches that not only enhance performance but also maintain low computational complexity.
In this study, we propose Kernel Least Squares (KLS) for linear transformation between semantic spaces. In our comprehensive analysis involving three intrinsic and two extrinsic experiments across six languages from three different language families and a comparative evaluation with nine different linear transformation methods, we demonstrate the superior performance of KLS. Our results show that the proposed method significantly improves word translation accuracy, thereby standing out as the most efficient method for transforming only the source semantic space.

Accession Number: WOS:001307840300018

Conference Title: 27th International Conference on Text, Speech, and Dialogue (TSD)

Conference Date: SEP 09-13, 2024

Conference Location: Brno, CZECH REPUBLIC

ISSN: 2945-9133

eISSN: 1611-3349

ISBN: 978-3-031-70562-5; 978-3-031-70563-2

Record 264 of 274

Title: ANALYSIS OF BOUNDARY CONDITIONS PROPERTIES IN THE SPH METHOD

Author(s): Nemecek, J (Nemecek, J.); Halada, T (Halada, T.); Benes, L (Benes, L.)

Edited by: Simurda D; Bodnar T

Source: TOPICAL PROBLEMS OF FLUID MECHANICS 2024 **Book Series:** Topical Problems of Fluid Mechanics **Pages:** 150-157 **DOI:** 10.14311/TPFM.2024.020 **Published Date:** 2024

Abstract: This article deals with analysis of boudary conditions for meshfree Smoothed particle hydrodynamics method (SPH). Two variants of boundary condition were analyzed, Dynamic boundary condition (DBC) and Boundary integral (BI), on one simple case. Furthermore we introduce a possible shape of an additional term for BI formulation, which models the tangential interaction of the fluid with boundary. A comparison between BI with additional term and DBC is made using the example of horizontal motion of fluid particle over an infinite wall.

Accession Number: WOS:001242655400020

Conference Title: Conference on Topical Problems of Fluid Mechanics

Conference Date: FEB 21-23, 2024

Conference Location: Czech Acad Sci, Inst Thermomechan, Prague, CZECH REPUBLIC

Conference Sponsors: Czech Tech Univ, Fac Mech Engn, Dept Tech Math, Univ Toulon, Imath, ERCOFTAC, Czech Pilot Ctr

Conference Host: Czech Acad Sci, Inst Thermomechan

ISSN: 2336-5781

ISBN: 978-80-87012-88-8

Record 265 of 274

Title: Comparison of Spine Segmentation Algorithms on Clinical Data from Spectral CT of Patients with Multiple Myeloma

Author(s): Nohel, M (Nohel, Michal); Jakubicek, R (Jakubicek, Roman); Blazkova, L (Blazkova, Lenka); Valek, V (Valek, Vlastimil); Dostal, M (Dostal, Marek); Ourednicek, P (Ourednicek, Petr); Chmelik, J (Chmelik, Jiri)

Edited by: Badnjevic A; Pokvic LG

Source: MEDICON 2023 AND CMBEBIH 2023, VOL 1 **Book Series:** IFMBE Proceedings **Volume:** 93 **Pages:** 309-317 **DOI:** 10.1007/978-3-031-49062-0_34 **Published Date:** 2024

Abstract: This article presents an evaluation of spine segmentation models using clinical data obtained from multiple myeloma patients. The performance of the models is compared based on the classical Dice score. The results show that the Payer and nnU-Net models show the highest level of similarity in segmentation. However, when it comes to the challenging task of segmenting cervical vertebrae, the Payer algorithm provides more accurate results. On the other hand, the nnU-Net model achieves better results in cases of extensive vertebral deformation. We also observed that convolutional neural networks have problems in segmenting metal surgical implants. Research highlights the strengths and weaknesses of different models and can help select appropriate segmentation algorithms for specific clinical scenarios.

Accession Number: WOS:001261436400034

Conference Title: Mediterranean Conference on Medical and Biological Engineering and Computing (MEDICON) and International Conference on Medical and Biological Engineering (CMBEBIH)

Conference Date: SEP 14-16, 2023

Conference Location: Sarajevo, BOSNIA & HERCEG

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Jakubicek, Roman	D-3622-2018	
Nohel, Michal	GQJ-8442-2022	
Dostal, Marek	HNS-2824-2023	
Chmelik, Jiri	H-9359-2017	0000-0001-9950-6279

ISSN: 1680-0737

ISBN: 978-3-031-49061-3; 978-3-031-49062-0

Record 266 of 274

Title: Techniques for Efficient Fourier Transform Computation in Ultrasound Simulations

Author(s): Olsak, O (Olsak, Ondrej); Jaros, J (Jaros, Jiri)

Book Group Author(s): Assoc Computing Machinery

Source: PROCEEDINGS OF THE 33RD INTERNATIONAL SYMPOSIUM ON HIGH-PERFORMANCE PARALLEL AND DISTRIBUTED COMPUTING, HPDC 2024 **DOI:** 10.1145/3625549.3658825 **Published Date:** 2024

Abstract: Noninvasive ultrasound surgeries represent a rapidly growing field in medical applications. Preoperative planning often relies on computationally expensive ultrasound simulations. This paper explores methods to accelerate these simulations by reducing the computation time of the Fourier transform, which is an integral part of the simulation in the k-Wave toolbox. Two experiments and their results will be presented. The first investigates substituting the standard Fast Fourier Transform (FFT) with a Sparse Fourier Transform (SFT). The second approach utilises filtering of the frequency spectrum, inspired by image compression algorithms. The aim of both experiments is to find a suitable method for accelerating the Fourier transform while utilising the sparsity of the spectrum in acoustic pressure. Our findings show that filtering offers significantly better results in terms of computation error, leading to a substantial reduction in overall simulation runtime.

Accession Number: WOS:001305813000032

Conference Title: 33rd International Symposium on High-Performance Parallel and Distributed Computing (HPDC)

Conference Date: JUN 03-07, 2024

Conference Location: Pisa, ITALY

Conference Sponsors: ACM SIGARCH, E4 COMPUTER ENGN, VAST, CORNELIS NETWORKS, NEC Laboratories Amer

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Record 267 of 274

Title: PROBING SELF-SUPERVISED LEARNING MODELS WITH TARGET SPEECH EXTRACTION<bold> </bold>

Author(s): Peng, J (Peng, Junyi); Delcroix, M (Delcroix, Marc); Ochiai, T (Ochiai, Tsubasa); Plchot, O (Plchot, Oldrich); Ashihara, T (Ashihara, Takanori); Araki, S (Araki, Shoko); Cernocky, J (Cernocky, Jan)

Book Group Author(s): IEEE

Source: 2024 IEEE INTERNATIONAL CONFERENCE ON ACOUSTICS, SPEECH, AND SIGNAL PROCESSING WORKSHOPS, ICASSPW 2024 **Pages:** 535-539 **DOI:** 10.1109/ICASSPW62465.2024.10627502 **Published Date:** 2024

Abstract: Large-scale pre-trained self-supervised learning (SSL) models have shown remarkable advancements in speech-related tasks. However, the utilization of these models in complex multi-talker scenarios, such as extracting a target speaker in a mixture, is yet to be fully evaluated. In this paper, we introduce target speech extraction (TSE) as a novel downstream task to evaluate the feature extraction capabilities of pre-trained SSL models. TSE uniquely requires both speaker identification and speech separation, distinguishing it from other tasks in the Speech processing Universal PERformance Benchmark (SUPERB) evaluation. Specifically, we propose a TSE downstream model composed of two lightweight task-oriented modules based on the same frozen SSL model. One module functions as a speaker encoder to obtain target speaker information from an enrollment speech, while the other estimates the target speaker's mask to extract its speech from the mixture. Experimental results on the Libri2mix datasets reveal the relevance of the TSE downstream task to probe SSL models, as its performance cannot be simply deduced from other related tasks such as speaker verification and separation.<bold> </bold>

Accession Number: WOS:001307820800146

Conference Title: 49th IEEE International Conference on Acoustics, Speech, and Signal Processing (ICASSP)

Conference Date: APR 14-19, 2024

Conference Location: Seoul, SOUTH KOREA

Conference Sponsors: Inst Elect & Elect Engineers, Inst Elect & Elect Engineers Signal Proc Soc

ISBN: 979-8-3503-7452-0; 979-8-3503-7451-3

Record 268 of 274

Title: A Comparison of Logic Extraction Methods in Hardware-Translated Neural Networks

Author(s): Schmidt, J (Schmidt, Jan); Fiser, P (Fiser, Petr); Skrbek, M (Skrbek, Miroslav)

Edited by: Deniziak S; Sitek P; Jenihhin M; Steininger A; Scholzel M; Mrazek V

Source: 2024 27TH INTERNATIONAL SYMPOSIUM ON DESIGN & DIAGNOSTICS OF ELECTRONIC CIRCUITS & SYSTEMS, DDECS **Book Series:** IEEE International Symposium on Design and Diagnostics of Electronic Circuits & Systems **Pages:** 86-91 **DOI:** 10.1109/ENC60556.2023.10508902 **Published Date:** 2024

Abstract: Small quantized neural networks with strong requirements on throughput and latency can be translated into logic circuits and synthesized by logic design tools. With networks having no state (memory), the circuits are combinational. To capture the function of the network (or a part of it) as a logic function, two approaches have been taken. The first one observes the inputs and outputs, while the network predicts a training set, and uses them directly as specification. The response to activation values that have not occurred in the training set remains unspecified. The other approach uses a complete set of activation values at the input of the examined part. We measured accuracy, the influence of logic minimization, and their impact on the final synthesized circuit on dense neural networks in different stages of low-magnitude pruning on the MNIST and JSC datasets. The results show that the first method can be used for functions with fan-in below 10-12 while not working against generalization. We also document the quantitative changes in quantized networks.

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Conference Title: 27th International Symposium on Design & Diagnostics of Electronic Circuits & Systems (DDECS)

Conference Date: APR 03-05, 2024

Conference Location: Kielce, POLAND

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Skrbek, Miroslav	D-9323-2016	

ISSN: 2334-3133

ISBN: 979-8-3503-5934-3

Record 269 of 274

Title: Modernized Training of U-Net for Aerial Semantic Segmentation

Author(s): Straka, J (Straka, Jakub); Gruber, I (Gruber, Ivan)

Book Group Author(s): IEEE Comp Soc

Source: 2024 IEEE WINTER CONFERENCE ON APPLICATIONS OF COMPUTER VISION WORKSHOPS, WACVW 2024 **Book Series:** IEEE Winter Conference on Applications of Computer Vision Workshops **Pages:** 785-793 **DOI:** 10.1109/WACVW60836.2024.00091 **Published Date:** 2024

Abstract: In this paper, we propose an improved training protocol of U-Net architecture for the semantic segmentation of aerial images. We test our approach on the challenging FLAIR #2 dataset. We present an extensive ablation study on the influence of different approach components on the overall performance. The ablation study includes a comparison of different model backbones, image augmentations, learning rate schedulers, loss functions, and training procedures. We additionally propose a two-stage training procedure and evaluate different options for the model ensemble. Based on the results we design the final setup of the model training protocol. This final setup decreases the relative error by approximately 18% and achieves mIoU equal to 0.641, which is a new state-of-the-art result. Our code is available at: https://github.com/strakaj/U-Net-for-remote-sensing.

Accession Number: WOS:001223022200092

Conference Title: IEEE/CVF Winter Conference on Applications of Computer Vision (WACV)

Conference Date: JAN 04-08, 2024

Conference Location: Waikoloa, HI

Conference Sponsors: IEEE, CVF, IEEE Comp Soc

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ISBN: 979-8-3503-7028-7; 979-8-3503-7071-3

Record 270 of 274

Title: Towards Evaluating Policy Optimisation Agents Using Algorithmic Intelligence Quotient Test

Author(s): Vadinsky, O (Vadinsky, Ondrej); Zeman, P (Zeman, Petr)

Edited by: Nowaczyk S; Biecek P; Chung NC; Vallati M; Skruch P; Jaworek-Korjakowska J; Parkinson S; Nikitas A; Atzmuller M; Kliegr T; Schmid U; Bobek S; Lavrac N; Peeters M; VanDierendonck R; Robben S; Mercier-Laurent E; Kayakutlu G; Owoc ML; Mason K; Wahid A; Bruno P; Calimeri F; Cauteruccio F; Terracina G; Wolter D; Leidner JL; Kohlhase M; Dimitrova V

Source: ARTIFICIAL INTELLIGENCE-ECAI 2023 INTERNATIONAL WORKSHOPS, PT 1, XAI3, TACTIFUL, XI-ML, SEDAMI, RAAIT, AI4S, HYDRA, AI4AI, 2023 **Book Series:** Communications in Computer and Information Science **Volume:** 1947 **Pages:** 435-451 **DOI:** 10.1007/978-3-031-50396-2_25 **Published Date:** 2024

Abstract: With the advent of more powerful AI systems, the issue of theoretically well-founded and more robust methods for general evaluation of intelligence in (not only) artificial systems increases in importance. The Algorithmic Intelligence Quotient Test (AIQ test) is an example of a reasonably well-founded yet practically feasible test of intelligence. Deep Reinforcement Learning offers a powerful framework that enables artificial agents to learn how to act in unknown environments of realistic complexities. Vanilla Policy Gradient (VPG) and Proximal Policy Optimisation (PPO) are two examples of model-free on-policy deep reinforcement learning agents. In this paper, a computational experiment with the AIQ test is conducted that evaluates VPG and PPO agents and compares them to classical off-policy Q-learning. An initial analysis of the results indicates that while the maximum AIQ achieved is comparable for the tested agents given sufficient training time, large differences show with short training times. Corresponding to previous research, on-policy methods have lower starting positions than off-policy methods, and PPO learns faster than VPG. This further depends on steps-per-epoch parameter setting of PPO and VPG agents. These findings indicate the utility of the AIQ test as an AI evaluation method.

Accession Number: WOS:001259329400025

Conference Title: 26th European Conference on Artificial Intelligence (ECAI)

Conference Date: SEP 30-OCT 04, 2023

Conference Location: Krakow, POLAND

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Record 271 of 274

Title: A Component of Stimulus-Frequency Otoacoustic Emissions Evoked due to Perturbation of Nonlinear Force in a Cochlear Model

Author(s): Vencovsky, V (Vencovsky, Vaclav); Klimes, O (Klimes, Ondrej); Vetesník, A (Vetesnik, Ales)

Edited by: Dong W; Epp B

Source: NONLINEARITY AND HEARING: ADVANCES IN THEORY AND EXPERIMENT **Book Series:** AIP Conference Proceedings **Volume:** 3062 **Article Number:** 030014 **DOI:** 10.1063/5.0189467 **Published Date:** 2024

Abstract: Stimulus-frequency otoacoustic emissions (SFOAEs) are evoked by a single tone presented into the ear. The emissions are generated by reflection of a forward traveling wave (TW) on localized irregularities in the impedance along the basilar membrane (BM). The strongest wavelets are reflected from the place where the TW reaches its largest amplitude. Since the irregularities are localized in fixed places along the basilar membrane, the latency of the SFOAE phase can be used to estimate delay of cochlear filters. We used an iterative approach of Shera et al. [JASA (2005) 118:287-313] to obtain an analytical solution for SFOAEs in a nonlinear two-dimensional cochlear model. The solution allowed for decomposition of a reflection component and a component due to perturbation of the nonlinear force. The nonlinear force which in the smooth cochlea may reflect the forward TW backwards [Talmadge et al., JASA (2000) 108, 2911-2931], is perturbed due to irregularities. The perturbed nonlinear force in the model generates an SFOAE component with latency comparable with the latency of the component due to reflection. This means that although the component is evoked due to nonlinear force, it has a comparable (long) latency to the SFOAE component due to reflection. The amplitude of this component due to perturbation of the nonlinear force grows as the amplitude of irregularities increases. In addition, the component amplitude also grows with the tone intensity. The growth is determined by the amplitude of the nonlinear force. It is almost cubic at the lowest intensities and quickly saturates at levels above about 40 dB SPL (the intensity is determined by the position of the compressive nonlinearity in the input/output function of the basilar membrane displacement). An interesting result is that the nonlinear component partly cancels the reflection component because its phase is shifted by approximately 0.5 cycles, independent of stimulus intensity and frequency. As the level increases, the component due to perturbation reaches an amplitude comparable to the component due to coherent reflection, especially in the portions of SFOAEs with the longest latencies. The destructive interference between the components due to perturbation of the nonlinear force and coherent reflection emphasizes shorter latency wavelets in the overall SFOAEs as stimulus intensity increases and contributes to the saturation of SFOAE amplitude reported, for example, in human experimental data of Abdala and Kalluri [JASA (2017) 142, 812-824].

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Conference Title: 14th International Mechanics of Hearing (MoH) Workshop

Conference Date: JUL 24-29, 2022

Conference Location: Helsingor, DENMARK

Conference Sponsors: Tech Univ Denmark, Loma Linda Univ, Natl Inst Deafness & Commun Disorders, Carlsberg Fdn, GN Fdn, Google, HEAD Genuit Stiftung, Mech Hearing 2017, Novo Nordisk Fdn, Real Labs, Thorlabs, William Demant Fonden

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Record 272 of 274

Title: RESET: Relational Similarity Extension for V3C1 Video Dataset

Author(s): Vesely, P (Vesely, Patrik); Peska, L (Peska, Ladislav)

Edited by: Rudinac S; Hanjalic A; Liem C; Worring M; Jonsson BP; Liu B; Yamakata Y

Source: MULTIMEDIA MODELING, MMM 2024, PT V **Book Series:** Lecture Notes in Computer Science **Volume:** 14565 **Pages:** 1-14 **DOI:** 10.1007/978-3-031-56435-2_1 **Published Date:** 2024

Abstract: Effective content-based information retrieval (IR) is crucial across multimedia platforms, especially in the realm of videos. Whether navigating a personal home video collection or browsing a vast streaming service like YouTube, users often find that a simple metadata search falls short of meeting their information needs. Achieving a reliable estimation of visual similarity holds paramount significance for various IR applications, such as query-by-example, results clustering, and relevance feedback. While many pre-trained models exist for this purpose, they often mismatch with human-perceived similarity leading to biased retrieval results. Up until now, the practicality of fine-tuning such models has been hindered by the absence of suitable datasets.

This paper introduces RESET: RElational Similarity Evaluation dataseT. RESET contains over 17,000

similarity annotations for query-candidate-candidate triples of video keyframes taken from the publicly available V3C1 video collection. RESET addresses both close and distant triplets within the realm of unconstrained V3C1 imagery and two of its compact sub-domains: wedding and diving. Offering fine-grained similarity annotations along with their context, re-annotations by multiple users, and similarity estimations from 30 pre-trained models, RESET serves dual purposes. It facilitates the evaluation of novel visual embedding models w.r.t. similarity preservation and provides a resource for fine-tuning visual embeddings to better align with human-perceived similarity. The dataset is available from https://osf.io/ruh5k.

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Conference Title: 30th International Conference on Multimedia Modeling (MMM)

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Conference Location: Amsterdam, NETHERLANDS

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Record 273 of 274

Title: Two-Tone Suppression and Power Balance in a 2D Nonlinear Cochlear Model

Author(s): Vetesník, A (Vetesnik, Ales); Klimes, O (Klimes, Ondrej); Vencovsky, V (Vencovsky, Vaclav)

Edited by: Dong W; Epp B

Source: NONLINEARITY AND HEARING: ADVANCES IN THEORY AND EXPERIMENT **Book Series:** AIP Conference Proceedings **Volume:** 3062 **Article Number:** 060013 **DOI:** 10.1063/5.0189281 **Published Date:** 2024

Abstract: Two-tone suppression (TTS) is the nonlinear phenomenon in which cochlear responses in the region most sensitive to a probe tone are reduced if a second tone (suppressor) of different frequency is simultaneously presented. TTS occurs due to saturation of mechanoelectrical transducers (MET) in the outer hair cells. The nonlinear dependence of MET channel conductance is the main cause of nonlinearity in cochlear amplification. Although the cochlear amplifier primarily acts locally, it influences distant fluid coupled parts of the basilar membrane (BM). The question therefore arises, how the fluid coupling contributes to the TTS. To answer this question, TTS was analysed using a 2D nonlinear cochlear model in two cases: for a suppressor of higher frequency and for a suppressor of lower frequency than the probe tone. It is shown that the BM-BM hydrodynamical coupling redistributed the excess of the power generated by the OHC electromechanical feedback force. It is also shown that the short-range part of the BM-BM coupling plays an important role in power balance along the BM. Moreover, it turned out from the model simulations that the suppression by a low-frequency suppressor causes a basal shift of the amplitude maximum and affects the phase of the BM stationary response. In contrast, the suppression by a high-frequency suppressor does not significantly affect the BM response phase; it flattens the amplitude of the BM stationary response, which leads to an apical shift of the amplitude maximum.

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Conference Title: 14th International Mechanics of Hearing (MoH) Workshop

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Conference Sponsors: Tech Univ Denmark, Loma Linda Univ, Natl Inst Deafness & Commun Disorders, Carlsberg Fdn, GN Fdn, Google, HEAD Genuit Stiftung, Mech Hearing 2017, Novo Nordisk Fdn, Real Labs, Thorlabs, William Demant Fonden

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Record 274 of 274

Title: Written Term Detection Improves Spoken Term Detection

Author(s): Yusuf, B (Yusuf, Bolaji); Saraçlar, M (Saraclar, Murat)

Source: IEEE-ACM TRANSACTIONS ON AUDIO SPEECH AND LANGUAGE PROCESSING **Volume:** 32 **Pages:** 3213-3223 **DOI:** 10.1109/TASLP.2024.3407476 **Published Date:** 2024

Abstract: End-to-end (E2E) approaches to keyword search (KWS) are considerably simpler in terms of training and indexing complexity when compared to approaches which use the output of automatic speech recognition (ASR) systems. This simplification however has drawbacks due to the loss of modularity. In particular, where ASR-based KWS systems can benefit from external unpaired text via a language model, current formulations of E2E KWS systems have no such mechanism. Therefore, in this paper, we propose a multitask training objective which allows unpaired text to be integrated into E2E KWS without complicating indexing and search. In addition to training an E2E KWS model to retrieve text queries from spoken documents, we jointly train it to retrieve text queries from masked written documents. We show empirically that this approach can effectively leverage unpaired text for KWS, with significant improvements in search performance across a wide variety of languages. We conduct analysis which indicates that these improvements are achieved because the proposed method improves document representations for words in the unpaired text. Finally, we show that the proposed method can be used for domain adaptation in settings where in-domain paired data is scarce or nonexistent.

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