Close

Web of Science
Page 1 (Records 1 -- 50)
[1 | 2 | 3 | 4 | 5]

Record 1 of 235

Title: We just estimated twenty million fiscal multipliers

Author(s): Capek, J (Capek, Jan); Cuaresma, JC (Crespo Cuaresma, Jesus)

Source: OXFORD BULLETIN OF ECONOMICS AND STATISTICS **DOI:** 10.1111/obes.12351 **Early Access Date:** DEC 2019

Abstract: We analyse the role played by data and specification choices as determinants of the size of the fiscal multipliers obtai autoregressive models. The results, based on over twenty million fiscal multipliers estimated for European countries, indicate t modelling choices have a significant effect on the size and precision of fiscal multiplier estimates. In addition to the structural s these modelling choices include the definition of spending and taxes, the national accounts system employed, the use of partic measures, or whether data are smoothed prior to estimation. The cumulative effects of such arguably innocuous methodologic change in the spending multipliers of as much as 0.4 points.

Accession Number: WOS:000503252900001

ISSN: 0305-9049

eISSN: 1468-0084

Record 2 of 235

Title: Highly frustrated magnetism in relativistic d(4) Mott insulators: Bosonic analog of the Kitaev honeycomb model

Author(s): Chaloupka, J (Chaloupka, Jiri); Khaliullin, G (Khaliullin, Giniyat)

Source: PHYSICAL REVIEW B **Volume:** 100 **Issue:** 22 **Article Number:** 224413 **DOI:** 10.1103/PhysRevB.100.224413 **Published:** D

Abstract: We study the orbitally frustrated singlet-triplet models that emerge in the context of spin-orbit coupled Mott insulator configuration. In these compounds, low-energy magnetic degrees of freedom can be cast in terms of three-flavor "triplon" oper transitions between spin-orbit entangled J = 0 ionic ground state and excited J = 1 levels. In contrast to a conventional, flavor-is models, spin-orbit entangled triplon interactions are flavor-and-bond selective and thus highly frustrated. In a honeycomb latti with the Kitaev spin model-an infinite number of conserved quantities, no magnetic condensation, and spin correlations being However, due to the bosonic nature of triplons, there are no emergent gapless excitations within the spin gap, and the ground s paramagnet of dense triplon pairs with no long-range entanglement. Using exact diagonalization, we study the bosonic Kitaev r extensions, which break exact symmetries of the model and allow magnetic condensation of triplons. Possible implications for oxides are discussed.

Accession Number: WOS:000502781200005

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eISSN: 2469-9969

Record 3 of 235

Title: Enzymatic Preparation of 2 '-5 ',3 '-5 '-Cyclic Dinucleotides, Their Binding Properties to Stimulator of Interferon Genes Ada Structure/Activity Correlations

Author(s): Novotna, B (Novotna, Barbora); Vanekova, L (Vanekova, Lenka); Zavrel, M (Zavrel, Martin); Budesinsky, M (Budesinsky Milan); Smola, M (Smola, Miroslav); Gutten, O (Gutten, Ondrej); Tehrani, ZA (Tehrani, Zahra Aliakbar); Polidarova, MP (Polidarova Brazdova, A (Brazdova, Andrea); Liboska, R (Liboska, Radek); Stepanek, I (Stepanek, Ivan); Vavrina, Z (Vavrina, Zdenek); Jandusi Nencka, R (Nencka, Radim); Rulisek, L (Rulisek, Lubomir); Boura, E (Boura, Even); Brynda, J (Brynda, Jiri); Pav, O (Pav, Ondrej); E

Source: JOURNAL OF MEDICINAL CHEMISTRY **Volume:** 62 **Issue:** 23 **Pages:** 10676-10690 **DOI:** 10.1021/acs.jmedchem.9b01062

Abstract: Cyclic dinucleotides are second messengers in the cyclic GMP-AMP synthase (cGAS)-stimulator of interferon genes (ST important role in recognizing tumor cells and viral or bacterial infections. They bind to the STING adaptor protein and trigger ex TANK binding kinase 1 (TBK1)/interferon regulatory factor 3 (IRF3) and inhibitor of nuclear factor-kappa B (I kappa B) kinase (IK kappa B) signaling cascades. In this work, we describe an enzymatic preparation of 2'-5',3'-5'-cyclic dinucleotides (2'3'CDNs) wi synthases (cGAS) from human, mouse, and chicken. We profile substrate specificity of these enzymes by employing a small libra triphosphate (NTP) analogues and use them to prepare 33 2'3'CDNs. We also determine affinity of these CDNs to five different S and biochemical assays and describe properties needed for their optimal activity toward all STING haplotypes. Next, we study t chemokine induction by human peripheral blood mononuclear cells (PBMCs) and evaluate their cytotoxic effect on monocytes. crystal structures of two new CDNs bound to STING protein and discuss structure-activity relationship by using quantum and m (QM/MM) computational modeling.

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PubMed ID: 31715099

Author Identifiers:

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ISSN: 0022-2623

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Record 4 of 235

Title: Atomistic simulation of carbohydrate-protein complex formation: Hevein-32 domain

Author(s): Solanke, CO (Solanke, Charles Oluremi); Trapl, D (Trapl, Dalibor); Sucur, Z (Sucur, Zoran); Mareska, V (Mareska, Vaclav Spiwok, V (Spiwok, Vojtech)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 18918 **DOI:** 10.1038/s41598-019-53815-w **Published:** DEC 12 2019

Abstract: Interactions between proteins and their small molecule ligands are of great importance for the process of drug design molecular dynamics simulation of systems containing hevein domain (HEV32) with N-acetylglucosamine mono-, di- or trisaccha molecules were placed outside the binding site. Three of six simulations (6 x 2 mu s) led to binding of a carbohydrate ligand into agreement with the experimentally determined structure. Unbinding was observed in one simulation (monosaccharide). There intermediates of binding for mono and disaccharide. Trisaccharide binding was initiated by formation of carbohydrate-aromati results indicate that binding of ligands followed the model of conformational selection because the conformation of the protein observed before the binding. This study extends the concept of docking by dynamics on carbohydrate-protein interactions.

Accession Number: WOS:000502726800001

PubMed ID: 31831756

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Record 5 of 235

Title: Designing modular 3D printed reinforcement of wound composite hollow beams with semidefinite programming

Author(s): Tyburec, M (Tyburec, M.); Zeman, J (Zeman, J.); Novak, J (Novak, J.); Leps, M (Leps, M.); Plachy, T (Plachy, T.); Poul, R

Source: MATERIALS & DESIGN **Volume:** 183 **Article Number:** UNSP 108131 **DOI:** 10.1016/j.matdes.2019.108131 **Published:** DEC

Abstract: Fueled by their excellent stiffness-to-weight ratio and the availability of mature manufacturing technologies, filament reinforced polymers represent ideal materials for thin-walled laminate structures. However, their strong anisotropy reduces stru instabilities under shear and buckling. Increasing laminate thickness degrades weight and structural efficiencies and the applic is often uneconomical and labor-intensive. In this contribution, we introduce a convex linear semidefinite programming formul optimization to design an efficient non-uniform lattice-like internal structure. The internal structure not only reduces the effect in the increase of the fundamental free-vibration eigen frequency, but also keeps weight low, secures manufacturability using c dimensional printers, and withstands the loads induced during the production process. We showcase a fully-automatic procedu prototype manufacturing, and verification of a simply-supported composite machine tool component, including validation with results confirm that the 3D-printed optimized internal structure almost doubles the fundamental free-vibration eigen frequency working frequency of the machine tool, even though the ratio between elastic properties of the carbon composite and the ABS exceeds two orders of magnitude. (C) 2019 The Authors. Published by Elsevier Ltd.

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Record 6 of 235

Title: Computational Modeling of the Ce@C-82 Metallofullerene Isomeric Composition

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

Source: ECS JOURNAL OF SOLID STATE SCIENCE AND TECHNOLOGY **Volume:** 8 **Issue:** 12 **Pages:** M118-M121 **DOI:** 10.1149/2.00 2019

Abstract: Relative populations of the IPR (isolated-pentagon-rule) isomers of Ce@C-82 under the high-temperature synthetic co the Gibbs energy based on characteristics from the density functional theory calculations (B3LYP/3-21G similar to SDD entropy to SDD energetics). In agreement with observation, Ce@C-2v(9)-C82 (major isomer) and Ce@C-s(c; 6)-C-82 (minor isomer) endo populated species. Their observed ratio is in the computational modeling reached at a temperature of about 1225 K (under a pr solubility of the isomers). (C) The Author(s) 2019. Published by ECS.

Accession Number: WOS:000500511200001

ISSN: 2162-8769

Record 7 of 235

Title: Experimental and Theoretical Studies of Preferential Solvation of 4-Nitroaniline and 4-Nitroanisole in an Amino Acid Ionic Solvents

Author(s): Aryafard, M (Aryafard, Meysam); Jahanshah, M (Jahanshah, Mohammadjavad); Harifi-Mood, AR (Harifi-Mood, Ali Reza Babak); Smatanova, IK (Smatanova, Ivana Kuta)

Source: JOURNAL OF CHEMICAL AND ENGINEERING DATA **Volume:** 64 **Issue:** 12 **Pages:** 5755-5764 **DOI:** 10.1021/acs.jced.9b007

Abstract: Amino acid ionic liquids (AAILs) are a new green class of ILs. Maximum wave numbers of 4-nitroaniline and 4-nitroanis solvatochromic method were calculated in binary mixtures of tetra butyl ammonium glycinate ([N-444][Gly]) with both protic a to understand the microsphere solvations and preferred solvents. These investigations showed that the effects of glycinate in [N hydrogen-bond basicity (beta) and polarizabihty (e), and they illustrated that normalized polarity (E-T(N)), pi*, and beta of [N-4 of molecular solvents. The preferential solvation model presented that the probes prefer to be solvated by either IL or mixed so (MD) simulations confirmed the preferential solvation model results and were used to analyze the microsphere solvation of dye the glycinate attend the microsphere solvation of 4-nitroaniline to have hydrogen bond interactions with amine group, but the for 4nitroanisole. Therefore, shift wavelengths of 4-nitroaniline in binary mixtures are noticeable, which were seen in experimer simulations were applied to understand the structural analysis of [N-4444][Gly] and solvent solvent interactions and it showed probabilities for hydrogen bond interactions between the glycinate and butanol. Finally, QM calculations confirmed both the ex simulation findings.

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Record 8 of 235

Title: SAT-Based Generation of Optimum Circuits with Polymorphic Behavior Support

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

Source: JOURNAL OF CIRCUITS SYSTEMS AND COMPUTERS **Volume:** 28 **Special Issue:** SI **Article Number:** 1940010 **DOI:** 10.1142/S0218126619400103 **Supplement:** 1 **Published:** DEC 1 2019

Abstract: This paper presents a method for generating optimum multi-level implementations of Boolean functions based on Sa Boolean Optimization (PBO) problems solving. The method is able to generate one or enumerate all optimum implementations gate types and gates costs can be arbitrarily specified. Polymorphic circuits represent a newly emerging computation paradigm structure is capable of performing two or more different intended functions, depending on instantaneous conditions in the targ this paper we propose the first method ever, generating provably size-optimal polymorphic circuits. Scalability and feasibility o by providing experimental results for all NPN-equivalence classes of four-input functions implemented in AND-Inverter and AND polymorphic behavior support being used and for all pairs of NPN-equivalence classes of three-input functions for polymorphic smaller benchmark circuits were synthesized optimally, both in standard and polymorphic logics.

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Record 9 of 235

Title: Gaussian Process Surrogate Models for the CMA Evolution Strategy

Author(s): Bajer, L (Bajer, Lukas); Pitra, Z (Pitra, Zbynek); Repicky, J (Repicky, Jakub); Holena, M (Holena, Martin)

Source: EVOLUTIONARY COMPUTATION **Volume:** 27 **Issue:** 4 **Pages:** 665-697 **DOI:** 10.1162/evco_a_00244 **Published:** DEC 2019

Abstract: This article deals with Gaussian process surrogate models for the Covariance Matrix Adaptation Evolutionary Strategy existing and two by the authors recently proposed models are presented. The work discusses different variants of surrogate mo on the benefits of employing the Gaussian process uncertainty prediction, especially during the selection of points for the evalu The experimental part of the article thoroughly compares and evaluates the five presented Gaussian process surrogate and six optimizers on the COCO benchmarks. The algorithm presented in most detail, DTS-CMA-ES, which combines cheap surrogate-m objective function evaluations in every iteration, is shown to approach the function optimum at least comparably fast and ofter art black-box optimizers for budgets of roughly 25-100 function evaluations per dimension, in 10- and less-dimensional spaces per dimension.

Accession Number: WOS:000500189000005

PubMed ID: 30540493

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Record 10 of 235

Title: Robustness and sensitivity analyses for stochastic volatility models under uncertain data structure

Author(s): Pospisil, J (Pospisil, Jan); Sobotka, T (Sobotka, Tomas); Ziegler, P (Ziegler, Philipp)

Source: EMPIRICAL ECONOMICS **Volume:** 57 **Issue:** 6 **Pages:** 1935-1958 **DOI:** 10.1007/s00181-018-1535-3 **Published:** DEC 2019

Abstract: In this paper, we perform robustness and sensitivity analysis of several continuous-time stochastic volatility (SV) mod process of market calibration. The analyses should validate the hypothesis on importance of the jump part in the underlying m of the long memory parameter is measured for the approximative fractional SV model (FSV). For the first time, the robustness o measured using bootstrapping methods on market data and Monte Carlo filtering techniques. In contrast to several other sensi SV models, the newly proposed methodology does not require independence of calibrated parameters-an assumption that is t practice. Empirical study is performed on a data set of Apple Inc. equity options traded in four different days in April and May 2 for Heston, Bates and approximative FSV models are provided.

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ISSN: 0377-7332

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Record 11 of 235

Title: Polymeric hollow fibers: A supercompact cooling of Li-ion cells

Author(s): Bohacek, J (Bohacek, Jan); Raudensky, M (Raudensky, Miroslav); Kroulikova, T (Kroulikova, Tereza); Karimi-Sibaki, E

Source: INTERNATIONAL JOURNAL OF THERMAL SCIENCES **Volume:** 146 **Article Number:** UNSP 106060 **DOI:** 10.1016/j.ijtherm DEC 2019

Abstract: An unconventional design of the heat exchanger has been introduced for conventional liquid cooled systems of batte vehicles (EVs). It is deemed unconventional, because only non-metallic materials are used, namely polydicyclopentadiene (PD and polymeric hollow fibers as coolant channels. The heat exchanger is lightweight, electrically non-conductive, durable, wear manufacturable. Very small in diameter (< 1 mm), the fibers were woven in a specific manner around a number of cylindrical Li- fibers' position was fixed in PDCPD processed during the reaction injection molding (RIM). In this study, the cooling performanc examined both numerically and in experiments. The findings of both approaches concur with each other. From the perspective the current prototype shows acceptable performance when compared to the standard exchangers on the market. The results p for promising design modifications.

Accession Number: WOS:000491874400036

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ISSN: 1290-0729

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Record 12 of 235

Title: Cross-lingual word analogies using linear transformations between semantic spaces

Author(s): Brychcin, T (Brychcin, Tomas); Taylor, S (Taylor, Stephen); Svoboda, L (Svoboda, Lukas)

Source: EXPERT SYSTEMS WITH APPLICATIONS **Volume:** 135 **Pages:** 287-295 **DOI:** 10.1016/j.eswa.2019.06.021 **Published:** NOV

Abstract: The ability to represent the meaning of words is one of the core parts of natural language understanding (NLU), with a machine translation, summarization, question answering, information retrieval, etc. The need for reasoning in multilingual con knowledge in cross-lingual systems has given rise to cross-lingual semantic spaces, which learn representations of words acros With growing attention to cross-lingual representations, it has became crucial to investigate proper evaluation schemes. The w has been one of the most common tools to evaluate linguistic relationships (such as male-female relationships or verb tenses) meaning representations. In this paper, we go beyond monolingual representations and generalize the word analogy task acros intrinsic evaluation tool for cross-lingual semantic spaces. Our approach allows examining cross-lingual projections and their i meaning. It helps to discover potential weaknesses or advantages of cross-lingual methods before they are incorporated into d We experiment with six languages within different language families, including English, German, Spanish, Italian, Czech, and C monolingual semantic spaces are transformed into a shared space using dictionaries of word translations. We compare several rank them for experiments with monolingual (no transformation), bilingual (one semantic space is transformed to another), an spaces are transformed onto English space) versions of semantic spaces. We show that tested linear transformations preserve r (word analogies) and lead to impressive results. We achieve average accuracy of 51.1%, 43.1%, and 38.2% for monolingual, bili

semantic spaces, respectively. (C) 2019 Elsevier Ltd. All rights reserved.

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Record 13 of 235

Title: Dynamics of mesoscopic polarization in the uniaxial tetragonal tungsten bronze (Sr(x)Bai(1-x))Nb2O6

Author(s): Buixaderas, E (Buixaderas, Elena); Kempa, M (Kempa, Martin); Svirskas, S (Svirskas, Sarunas); Kadlec, C (Kadlec, Chri Viktor); Savinov, M (Savinov, Maxim); Pasciak, M (Pasciak, Marek); Dec, J (Dec, Jan)

Source: PHYSICAL REVIEW B **Volume:** 100 **Issue:** 18 **Article Number:** 184113 **DOI:** 10.1103/PhysRevB.100.184113 **Published:** N

Abstract: The high-frequency dielectric behavior of uniaxial tungsten-bronze strontium barium niobate crystals with various Sr, ferroelectric and relaxor compositions, have been studied in a broad frequency range (10(4) to 10(13) Hz) and temperature inter thoroughly understand the evolution of the relaxation dynamics across the ferroelectric phase transition. The dielectric respon consists of three relaxations corresponding to polarization mechanisms related to several correlation lengths of mesoscopic or dissimilar behaviors with temperature, pointing out to their distinct nature. A temperature-dependent central mode at THz frec above 10 GHz are accompanied by the slowing down of a relaxation in the MHz range. This response reveals the complex mecha and supports the coexistence of displacive and order-disorder scenarios. Relaxor and ferroelectric compositions surprisingly re behavior within the frequency window used. However, relaxor crystals display relaxations at higher frequency because of the sr fluctuations and ferroelectric regions, which coexist in almost all the compositions. The presence of two different ferroelectric s agrees with the existence of several polarization mechanisms involved in the complex dielectric and ferroelectric response.

Accession Number: WOS:000498849400001

Author Identifiers:

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Kempa, Martin		0000-0002-5902-7780

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Record 14 of 235

Title: Chromosome Painting Facilitates Anchoring Reference Genome Sequence to Chromosomes In Situ and Integrated Karyot

Author(s): Simonikova, D (Simonikova, Denise); Nemeckova, A (Nemeckova, Alzbeta); Karafiatova, M (Karafiatova, Miroslava); U Brigitte); Swennen, R (Swennen, Rony); Dolezel, J (Dolezel, Jaroslav); Hribova, E (Hribova, Eva)

Source: FRONTIERS IN PLANT SCIENCE **Volume:** 10 **Article Number:** 1503 **DOI:** 10.3389/fpls.2019.01503 **Published:** NOV 20 20

Abstract: Oligo painting FISH was established to identify all chromosomes in banana (Musa spp.) and to anchor pseudomolecu sequence of Musa acuminata spp. malaccensis "DH Pahang" to individual chromosomes in situ. A total of 19 chromosome/chro painting probes were developed and were shown to be suitable for molecular cytogenetic studies in genus Musa. For the first ti diploid M. acuminata spp. malaccensis (A genome), M. balbisiana (B genome), and M. schizocarpa (S genome) from the Eumusa contributed to the evolution of edible banana cultivars, were established. This was achieved after a combined use of oligo paint previously developed banana cytogenetic markers. The density of oligo painting probes was sufficient to study chromosomal re well as on meiotic pachytene chromosomes. This advance will enable comparative FISH mapping and identification of chromos accompanied genome evolution and speciation in the family Musaceae.

Accession Number: WOS:000500980000001

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Record 15 of 235

Title: Magainin 2 and PGLa in Bacterial Membrane Mimics I: Peptide-Peptide and Lipid-Peptide Interactions

Author(s): Pachler, M (Pachler, Michael); Kabelka, I (Kabelka, Ivo); Appavou, MS (Appavou, Marie-Sousai); Lohner, K (Lohner, Kar
Pabst, G (Pabst, Georg)

Source: BIOPHYSICAL JOURNAL **Volume:** 117 **Issue:** 10 **Pages:** 1858-1869 **DOI:** 10.1016/j.bpj.2019.10.022 **Published:** NOV 19 2

Abstract: We addressed the onset of synergistic activity of the two well-studied antimicrobial peptides magainin 2 (MG2a) and F
of Gram-negative cytoplasmic membranes. Specifically, we coupled a joint analysis of smallangle x-ray and neutron scattering e
lipid vesicles in the presence of MG2a and L18W-PGLa to all-atom and coarse-grained molecular dynamics simulations. In agree
both peptides, as well as their equimolar mixture, were found to remain upon adsorption in a surface-aligned topology and to i
perturbation, as evidenced by membrane thinning and hydrocarbon order parameter changes in the vicinity of the inserted pep
particularly pronounced for the so-called synergistic mixture of 1:1 (mol/mol) L18W-PGLa/MG2a and cannot be accounted for b
membrane perturbations of two peptides individually. Our data are consistent with the formation of parallel heterodimers at cc
synergistic increase of dye leakage from vesicles. Our simulations further show that the heterodimers interact via salt bridges a
apparently makes them more stable than putatively formed antiparallel L18W-PGLa and MG2a homodimers. Moreover, dimeriz
leads to a relocation of the peptides within the lipid headgroup region as compared to the individual peptides. The early onset
and MG2a at low peptide concentrations consequently appears to be key to their synergistic dye-releasing activity from lipid ve

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PubMed ID: 31703802

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Record 16 of 235

Title: Interspecific introgression mediates adaptation to whole genome duplication

Author(s): Marburger, S (Marburger, Sarah); Monnahan, P (Monnahan, Patrick); Seear, PJ (Seear, Paul J.); Martin, SH (Martin, Sim
Jordan); Paajanen, P (Paajanen, Pirita); Bohutinska, M (Bohutinska, Magdalena); Higgins, JD (Higgins, James D.); Schmickl, R (S
(Yant, Levi)

Source: NATURE COMMUNICATIONS **Volume:** 10 **Article Number:** 5218 **DOI:** 10.1038/s41467-019-13159-5 **Published:** NOV 18 2

Abstract: Adaptive gene flow is a consequential phenomenon across all kingdoms. Although recognition is increasing, there is r
bidirectional gene flow mediates adaptation at loci that manage core processes. We previously discovered concerted molecular
members of the meiotic machinery controlling crossover number upon adaptation to whole-genome duplication (WGD) in Arab
conduct a population genomic study to test the hypothesis that adaptation to WGD has been mediated by adaptive gene flow b
lyrata. We find that A. lyrata underwent WGD more recently than A. arenosa, suggesting that pre-adapted alleles have rescued n
detect gene flow in the opposite direction at functionally interacting loci under the most extreme levels of selection. These data
gene flow allowed for survival after WGD, and that the merger of these species is greater than the sum of their parts.

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PubMed ID: 31740675

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ISSN: 2041-1723

Record 17 of 235

Title: Composite lymphoma of concurrent T zone lymphoma and large cell B cell lymphoma in a dog

Author(s): Matsuyama, A (Matsuyama, Arata); Bienzle, D (Bienzle, Dorothee); Richardson, D (Richardson, Danielle); Deravi, N (De
(Hwang, Mei-Hua); Darzentas, N (Darzentas, Nikos); Keller, SM (Keller, Stefan M.)

Source: BMC VETERINARY RESEARCH **Volume:** 15 **Issue:** 1 **Article Number:** 413 **DOI:** 10.1186/s12917-019-2154-8 **Published:** N

Abstract: Background Evolution of indolent to aggressive lymphoma has been described in dogs but is difficult to distinguish fr
of a second, clonally distinct lymphoma. Differentiation of these scenarios can be aided by next generation sequencing (NGS)-b
of lymphocyte antigen receptor genes. Case presentation An 8-year-old male intact Mastiff presented with generalized lymphad
with nodal T zone lymphoma (TZL) based on cytology, histopathology, immunohistochemistry and flow cytometry. Thirteen mo

presented with progressive lymphadenomegaly, and based on cytology and flow cytometry, a large B cell lymphoma (LBCL) wa based clonality testing confirmed the de novo development of a LBCL and the persistence of a TZL. Conclusions The occurrence neoplasms should be considered if patient features and tumor cytomorphology or immunophenotype differ among sequential clonality testing may provide conclusive evidence of two concurrent and distinct clonal lymphocyte populations, termed most lymphoma".

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PubMed ID: 31733649

eISSN: 1746-6148

Record 18 of 235

Title: Cophylogenetic relationships between Dactylogyrus (Monogenea) ectoparasites and endemic cyprinoids of the north-eas Mediterranean region

Author(s): Benovics, M (Benovics, Michal); Desdevises, Y (Desdevises, Yves); Sanda, R (Sanda, Radek); Vukic, J (Vukic, Jasna); Sir

Source: JOURNAL OF ZOOLOGICAL SYSTEMATICS AND EVOLUTIONARY RESEARCH **DOI:** 10.1111/jzs.12341 **Early Access Date:** N

Abstract: The study of host-parasite coevolution is one of the cornerstones of evolutionary biology. The majority of fish ectopar Dactylogyrus (Monogenea) exhibit a high degree of host specificity. Therefore, it is expected that their evolutionary history is pr evolutionary history of their cyprinoid fish hosts and the historical formation of the landmasses. In the present study, we used a investigate coevolutionary relationships between endemic Cyprinoidea (Cyprinidae and Leuciscidae) from selected regions in s respective Dactylogyrus species. A total of 49 Dactylogyrus species including endemic and non-endemic species were collected species in the Balkan and Apennine Peninsulas. However, 21 morphologically identified Dactylogyrus species exhibited differer from 2 to 28 variants per species) and some of them were recognized as cryptic species on the basis of phylogenetic reconstruct revealed several lineages of endemic and non-endemic Dactylogyrus species reflecting some morphological similarities or host based and event-based cophylogenetic methods, we found a significant coevolutionary signal between the phylogenies of para particular, statistically significant links were revealed between Dactylogyrus species of Barbini (Cyprinidae) and their hosts belc Aulopyge, Barbus and Luciobarbus. Additionally, a strong coevolutionary link was found between the generalist parasites D. ala and their hosts, and between Dactylogyrus species of Pachychilon (Leuciscidae) and their hosts. Cophylogenetic analyses sugg an important role in the evolutionary history of Dactylogyrus parasitizing endemic cyprinoids in southern Europe. We propose t phylogenetically related cyprinoid species in the Mediterranean area is a process facilitating the host switching of specific paras congeneric cyprinoids.

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Record 19 of 235

Title: Asteroid pairs: A complex picture

Author(s): Pravec, P (Pravec, P.); Fatka, P (Fatka, P.); Vokrouhlicky, D (Vokrouhlicky, D.); Scheirich, P (Scheirich, P.); Durech, J (Du (Scheeres, D. J.); Kusnirak, P (Kusnirak, P.); Hornoch, K (Hornoch, K.); Galad, A (Galad, A.); Pray, DP (Pray, D. P.); Krugly, YN (Krug (Burkhonovg, O.); Ehgamberdiev, SA (Ehgamberdiev, Sh A.); Pollockh, J (Pollockh, J.); Moskovitz, N (Moskovitz, N.); Thirouin, A (J. L.); Morales, N (Morales, N.); Husarik, M (Husarik, M.); Inasaridze, RY (Inasaridze, R. Ya); Oey, J (Oey, J.); Polishook, D (Polishoo Kucakova, H (Kucakova, H.); Vratil, J (Vratil, J.); Vilagi, J (Vilagi, J.); Gajdos, S (Gajdos, S.); Kornos, L (Kornos, L.); Veres, P (Veres, F N. M.); Hromakina, T (Hromakina, T.); Sergeyev, V (Sergeyev, V); Slyusarev, IG (Slyusarev, I. G.); Ayvazian, VR (Ayvazian, V. R.); Coc Gross, J (Gross, J.); Terrell, D (Terrell, D.); Colas, F (Colas, F.); Vachier, F (Vachier, F.); Slivan, S (Slivan, S.); Skiff, B (Skiff, B.); March (Ergashev, K. E.); Kim, DH (Kim, D-H); Aznarz, A (Aznarz, A.); Serra-Ricart, M (Serra-Ricart, M.); Behrend, R (Behrend, R.); Roy, R (R F.); Molotova, IE (Molotova, I. E.)

Source: ICARUS **Volume:** 333 **Pages:** 429-463 **DOI:** 10.1016/j.icarus.2019.05.014 **Published:** NOV 15 2019

Abstract: We studied a sample of 93 asteroid pairs, i.e., pairs of genetically related asteroids that are on highly similar heliocent elapsed since separation of pair members (i.e., pair age) that are between 7 x 10(3) yr and a few 10(6) yr. With photometric obse rotation periods P-1 for all the primaries (i.e., the larger members of asteroid pairs) and a sample of secondaries (the smaller pa absolute magnitude differences of the studied asteroid pairs that provide their mass ratios q. For a part of the studied pairs, we albedos and collected or estimated their taxonomic classifications. For 17 asteroid pairs, we also determined their pole positior obtained the spin poles for both pair components, we saw the same sense of rotation for both components and constrained the

spin vectors at the time of their separation. We found that the primaries of 13 asteroid pairs in our sample are actually binary or one or two bound, orbiting secondaries (satellites). As a by-product, we found also 3 new young asteroid clusters (each of them asteroids on highly similar heliocentric orbits). We compared the obtained asteroid pair data with theoretical predictions and d We found that 86 of the 93 studied asteroid pairs follow the trend of primary rotation period vs mass ratio that was found by Pra outliers, 3 appear insignificant (may be due to our uncertain or incomplete knowledge of the three pairs), but 4 are high mass ra unpredicted by the theory of asteroid pair formation by rotational fission. We discuss a (remotely) possible way that they could fission of flattened parent bodies followed by reshaping of the formed components. The 13 asteroid pairs with binary primaries systems that place important constraints on formation and evolution of asteroid pairs. We present two hypotheses for their forn having both bound and unbound secondaries could be "failed asteroid clusters", or they could be formed by a cascade primary studies are needed to reveal which of these two hypotheses for formation of the paired binary systems is real.

Accession Number: WOS:000481566200032

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Record 20 of 235

Title: A phylogenetic revision of the genus Hypnum: Towards completion

Author(s): Kucera, J (Kucera, Jan); Kuznetsova, OI (Kuznetsova, Oxana, I); Manukjanova, A (Manukjanova, Alzbeta); Ignatov, MS

Source: TAXON **DOI:** 10.1002/tax.12095 **Early Access Date:** NOV 2019

Abstract: The taxonomy of pleurocarpous mosses has long been based on a few key characters such as the presence or absence posture of the leaves. Molecular analyses performed in the past two decades have often challenged the traditional familial and these simple characters have evolved repeatedly. For nearly a century the genus Hypnum has been defined principally by the co with a short double costa, differentiated alar cells and the mostly procumbent growth form. Although several earlier treatments Hypnum in its traditional sense, none of them included a representative selection of the species on a worldwide basis. Therefor taxa that were attributed to the genus by the monographer H. Ando, and performed a molecular phylogenetic analysis using DN chloroplast loci and the nuclear ribosomal ITS region. The outcome of this analysis was a revision of the phylogenetic affinities we also matched more than 15 molecularly defined lineages of Hypnum s.l. to morphological characters and solved several nor Consequently, we suggest taxonomic and nomenclatural re-arrangements, which encompass the vast majority of taxa attribute contradict their known molecular affinities. We deliver additional support for some of the most recent delimitations of Hypnum refute the proposals for the segregation of the genera Lignocariosa and Insomniella, which can be accommodated in the existin Pseudohygrohypnum and Calohypnum, respectively. Similarly, we dispute the inclusion of Hypnum sauteri in Anacamptodon a establishment of a new genus for this species. Instead of placing Callicladium in the Hypnaceae and Jochenia in the Entodonta new families for these two genera. Finally, we propose three other new genera to accommodate (1) Hypnum circinale, (2) H. chr subchrysogaster, and (3) H. dieckii, respectively. The main diagnostic features of Hypnum in earlier treatments are shown to rep homoplastic characters, correlated with adaptation to the habitat conditions, such as the moisture content.

Accession Number: WOS:000496496700001

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Author	Web of Science ResearcherID	ORCID Number
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ISSN: 0040-0262

eISSN: 1996-8175

Record 21 of 235

Title: Germanane synthesis with simultaneous covalent functionalization: towards highly functionalized fluorescent germanan

Author(s): Sturala, J (Sturala, Jiri); Luxa, J (Luxa, Jan); Matejkova, S (Matejkova, Stanislava); Sofer, Z (Sofer, Zdenek); Pumera, M

Source: NANOSCALE **Volume:** 11 **Issue:** 41 **Pages:** 19327-19333 **DOI:** 10.1039/c9nr04081a **Published:** NOV 7 2019

Abstract: Monoelemental 2D-materials beyond graphene are attracting great attention. Although monolayer graphene or phosp
its layered 3D form, graphite or black phosphorus, by exfoliation of a large van der Waals crystal, this route is not suitable for th
germanene based materials due to the crystal structure and chemical properties of germanium. Unlike graphene or phosphore
prepared by chemical exfoliation from bulk Zintl phases - here represented by calcium germanide. We describe the exfoliation a
of calcium germanide, which yields layered germanium materials with alkyl or aryl groups. Different organic functional groups
germanane exhibit a very intense fluorescence in the blue region, which makes them prospective materials for further applicati
The described procedure for covalently functionalized germananes represents the way for the production of these materials.

Accession Number: WOS:000498821300060

PubMed ID: 31423498

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ISSN: 2040-3364

eISSN: 2040-3372

Record 22 of 235

Title: Detection and quantification of Melissococcus plutonius in honey bee workers exposed to European foulbrood in Czechia
qPCR, and barcode sequencing

Author(s): Sopko, B (Sopko, Bruno); Zitek, J (Zitek, Justyna); Nesvorna, M (Nesvorna, Marta); Markovic, M (Markovic, Martin); Ka
Titera, D (Titera, Dalibor); Erban, T (Erban, Tomas); Hubert, J (Hubert, Jan)

Source: JOURNAL OF APICULTURAL RESEARCH **DOI:** 10.1080/00218839.2019.1685148 **Early Access Date:** NOV 2019

Abstract: Melissococcus plutonius is the causative agent of European foulbrood (EFB), an important bacterial disease of honey
methods have been developed for the detection of this disease. Adult bees are not affected but spread M. plutonius among bee
diagnostic tool to detect EFB. Melissococcus plutonius detection based on conventional polymerase chain reaction (PCR) (16S
barcode sequencing of the 16S RNA V4 region in worker bees from colonies with and without clinical symptoms were compared
detection tools in terms of the presence/absence of clinical signs of the disease. The comparison of the PCR- and qPCR-based m
for confirmation of the disease in both colonies with and without clinical symptoms. Our results revealed that qPCR was more s
of clinical EFB than conventional PCR and that conventional PCR was better for general screening, including the screening of as
qPCR. Redundancy analyses (tbRDAs) of the microbiome composition showed that the detection limit-based qPCR of M. pluton
variability in the microbiome profiles of worker bees compared with that explained by clinical signs of the disease and PCR dete
of "secondary invaders" (Paenibacillus alvei and Enterococcus) was positively correlated with an increase in the profile of M. plu
microbiome, whereas Apibacter adventoris and Bartonella apis were negatively correlated. Both types of correlations were four

Accession Number: WOS:000495156300001

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ISSN: 0021-8839

eISSN: 2078-6913

Record 23 of 235

Title: Evolution of Termite Symbiosis Informed by Transcriptome-Based Phylogenies

Author(s): Bucek, A (Bucek, Ales); Sobotnik, J (Sobotnik, Jan); He, SL (He, Shulin); Shi, M (Shi, Mang); McMahon, DP (McMahon,
Edward C.); Roisin, Y (Roisin, Yves); Lo, N (Lo, Nathan); Bourguignon, T (Bourguignon, Thomas)

Source: CURRENT BIOLOGY **Volume:** 29 **Issue:** 21 **Pages:** 3728-+ **DOI:** 10.1016/j.cub.2019.08.076 **Published:** NOV 4 2019

Abstract: Termitidae comprises similar to 80% of all termite species [1] that play dominant decomposer roles in tropical ecosys
during termite evolution were the loss of cellulolytic gut protozoans in the ancestor of Termitidae and the subsequent gain in th
Macrotermitinae of fungal symbionts cultivated externally in "combs" constructed within the nest [4, 5]. How these symbiotic tr
unresolved. Phylo-genetic analyses of mitochondrial data previously suggested that Macrotermitinae is the earliest branching t
soon after by Sphaerotermitinae [6], which cultivates bacterial symbionts on combs inside its nests [7]. This has led to the hypo
an important evolutionary step in the loss of gut protozoa in ancestral termitids [8]. We sequenced genomes and transcriptome

reconstructed phylogenetic trees from up to 4,065 orthologous genes of 68 species. We found strong support for a novel sister-g the bacterial comb-building Sphaerotermitinae and fungus comb-building Macrotermitinae. This key finding indicates that com within Termitidae and that the creation of a comb-like "external rumen" involving bacteria or fungi may not have driven the los termitids, as previously hypothesized. Instead, associations with gut prokaryotic symbionts, combined with dietary shifts from substrates, may have played a more important role in this symbiotic transition. Our phylogenetic tree provides a platform for fu termite evolution and the evolution of symbiosis in this taxon.

Accession Number: WOS:000494940000035

PubMed ID: 31630948

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McMahon, Dino	F-7006-2012	0000-0003-1119-5299

ISSN: 0960-9822

eISSN: 1879-0445

Record 24 of 235

Title: Origin and Evolution of Diploid and Allopolyploid Camelina Genomes Were Accompanied by Chromosome Shattering

Author(s): Mandakova, T (Mandakova, Terezie); Pouch, M (Pouch, Milan); Brock, JR (Brock, Jordan R.); Al-Shehbaz, IA (Al-Shehb Martin A.)

Source: PLANT CELL **Volume:** 31 **Issue:** 11 **Pages:** 2596-2612 **DOI:** 10.1105/tpc.19.00366 **Published:** NOV 2019

Abstract: Complexes of diploid and polyploid species have formed frequently during the evolution of land plants. In false flax (C important hexaploid oilseed crop closely related to Arabidopsis (Arabidopsis thaliana), the putative parental species as well as species remained unknown. By using bacterial artificial chromosome-based chromosome painting, genomic in situ hybridizatic phylogenetics, we aimed to elucidate the origin and evolution of the polyploid complex. Genomes of diploid camelinas (Cameli laxa, n = 6; and Camelina neglecta, n = 6) originated from an ancestral n = 7 genome. The allotetraploid genome of Camelina rur from hybridization between diploids related to C. neglecta (n = 6, N-6) and C. hispida (n = 7, H), and the N subgenome has under polyploid fractionation. The allohexaploid genomes of C. sativa and Camelina microcarpa (n = 20, (NNH)-N-6-H-7) originated th an auto-allotetraploid C. neglecta-like genome (n = 13, (NN7)-N-6) and C. hispida (n = 7, H), and the three subgenomes have rem genome merger. Remarkably, the ancestral and diploid Camelina genomes were shaped by complex chromosomal rearrangem associated with human disorders and resulting in the origin of genome-specific shattered chromosomes.

Accession Number: WOS:000504310900011

PubMed ID: 31451448

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Lysak, Martin	D-2439-2014	0000-0003-0318-4194

ISSN: 1040-4651

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Record 25 of 235

Title: Structural and Electronic Properties of Oxidized and Amorphous Nanodiamond Surfaces with Covalently Grafted Polypyrr

Author(s): Matunov?, P (Matunova, Petra); Jir?sek, V (Jirasek, Vit); Rezek, B (Rezek, Bohuslav)

Source: PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS **Volume:** 256 **Issue:** 11 **Article Number:** 1900176 **DOI:** 10.1002 NOV 2019

Abstract: Diamond nanoparticles denoted as nanodiamonds (NDs) possess numerous beneficial material properties and are er applications. In this work, complexes of polypyrrole (PPy) organic dye covalently grafted to ND surfaces are investigated by ator theory (DFT) computations with a view to their structural and electronic properties. NDs terminated with oxygen, hydroxyl, carb amorphous carbon (a-C:H, a-C:O) have been considered. Thereby the theoretical model is brought close to real nanodiamonds. occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) and a favorable energetic level alignme observed for the majority of the oxidized NDs. This feature is also retained for NDs with amorphous surface layer. Excited states dependent DFT to analyze how the electronic configuration can promote dissociation of excitons, for instance in photovoltaic a

Accession Number: WOS:000503261600022

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eISSN: 1521-3951

Record 26 of 235

Title: Deciphering the Structural Basis of High Thermostability of Dehalogenase from Psychrophilic Bacterium Marinobacter sp.

Author(s): Chrast, L (Chrast, Lukas); Tratsiak, K (Tratsiak, Katsiaryna); Planas-Iglesias, J (Planas-Iglesias, Joan); Daniel, L (Daniel (Prudnikova, Tatyana); Brezovsky, J (Brezovsky, Jan); Bednar, D (Bednar, David); Smatanova, IK (Smatanova, Ivana Kuta); Chalo Radka); Damborsky, J (Damborsky, Jiri)

Source: MICROORGANISMS **Volume:** 7 **Issue:** 11 **Article Number:** 498 **DOI:** 10.3390/microorganisms7110498 **Published:** NOV

Abstract: Haloalkane dehalogenases are enzymes with a broad application potential in biocatalysis, bioremediation, biosensin haloalkane dehalogenase DmxA originating from the psychrophilic bacterium Marinobacter sp. ELB17 surprisingly possesses th (apparent melting temperature T-m,T-app = 65.9 degrees C) of all biochemically characterized wild type haloalkane dehalogena The enzyme was successfully expressed and its crystal structure was solved at 1.45 angstrom resolution. DmxA structure contai from known members of haloalkane dehalogenase family: (i) a unique composition of catalytic residues; (ii) a dimeric state mec and (iii) narrow tunnels connecting the enzyme active site with the surrounding solvent. The importance of narrow tunnels in s stability of DmxA enzyme was confirmed by computational protein design and mutagenesis experiments.

Accession Number: WOS:000502273600021

PubMed ID: 31661858

Author Identifiers:

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eISSN: 2076-2607

Record 27 of 235

Title: Quantum chemical calculations of P-31 NMR chemical shifts of P-donor ligands in platinum(II) complexes

Author(s): Sojka, M (Sojka, Martin); Necas, M (Necas, Marek); Tousek, J (Tousek, Jaromir)

Source: JOURNAL OF MOLECULAR MODELING **Volume:** 25 **Issue:** 11 **Article Number:** 329 **DOI:** 10.1007/s00894-019-4222-1 **Pu**

Abstract: This work aims to find the most suitable method that is practically applicable for the calculation of P-31 NMR chemica The influence of various all-electron and ECP basis sets, DFT functionals, and solvent effects on the optimized geometry was tes combinations of DFT functionals BP86, B3LYP, PBE0, TPSSh, CAM-B3LYP, and omega B97XD with all-electron basis sets 6-31G, 6- 6-311G(d,p), and TZVP and ECP basis sets SDD, LanL2DZ, and CEP-31G were used. Chemical shielding constants were then calcu B3LYP functionals in combination with the TZ2P basis. The magnitude of spin-orbit interactions was also evaluated.

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PubMed ID: 31656972

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eISSN: 0948-5023

Record 28 of 235

Title: Electric field determination from intensity ratio of N2+and N-2 bands: nonequilibrium transient discharges in pure nitroge

Author(s): Bilek, P (Bilek, Petr); Simek, M (Simek, Milan); Bonaventura, Z (Bonaventura, Zdenek)

Source: PLASMA SOURCES SCIENCE & TECHNOLOGY **Volume:** 28 **Issue:** 11 **Article Number:** 115011 **DOI:** 10.1088/1361-6595/a

Abstract: We developed an extension of the spectrometric method to estimate a reduced electric field (E/N), which is applicable plasmas. The method is based on the intensity ratio of the emission bands of the first negative system (FNS) of N2+<i and the se N-2. It uses the emission occurring in the wavelength interval 375?410 nm, which includes six SPS and two FNS bands. The choi guided by much simpler acquisition and processing of experimental data than the SPS(0, 0) and FNS(0, 0) pair that is typically u construct a kinetic model for pure molecular nitrogen, which determines the population of the upper states responsible for the Moreover, we perform sensitivity analysis of the kinetic model, which allows us to reveal the most significant processes for the i For these processes, we provide an in-depth review of the kinetic data that are available in the literature. We use the fact that th investigated contains bands to obtain three independent intensity ratios with sufficient signal-to-noise ratio ((FNS(0, 0)/SPS(0, 0)/SPS(2, 5)), which are usable for more accurate electric field determination. We also provide analytical formulas representing on E/N. Furthermore, we focus on different spectrometric representations of FNS and SPS bands, which also affect the precisio examine the FNS/SPS band profiles in terms of different rotational temperatures and instrumental functions. Finally, we propos enables the use of bandhead intensities in the intensity ratio dependencies, thus avoiding the need to evaluate integral band in spectra.

Accession Number: WOS:000499443300001

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Record 29 of 235

Title: Draft Genome Sequence of the Panton-Valentine Leucocidin-Producing Staphylococcus aureus Sequence Type 154 Strain Fatal Case of Necrotizing Pneumonia

Author(s): Indrakova, A (Indrakova, Adela); Maslanova, I (Maslanova, Ivana); Mrkva, O (Mrkva, Ondrej); Bendickova, K (Bendicko (Vrbovska, Veronika); Doskar, J (Doskar, Jiri); Pantucek, R (Pantucek, Roman)

Source: MICROBIOLOGY RESOURCE ANNOUNCEMENTS **Volume:** 8 **Issue:** 47 **Article Number:** UNSP e01299-19 **DOI:** 10.1128/M 2019

Abstract: Panton-Valentine leucocidin (PVL)-positive methicillin-resistant Staphylococcus aureus (MRSA) strains cause life-threa draft genome sequence of PVL-positive MRSA sequence type 154 (ST154) strain NRL 08/001, isolated from a fatal case of necroti consists of 2.9 Mb over 39 contigs and harbors novel composite island staphylococcal cassette chromosome mec element (SCC 2B&5.

Accession Number: WOS:000498050200007

PubMed ID: 31753953

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pantucek, Roman	P-6758-2014	0000-0002-3950-675X

ISSN: 2576-098X

Record 30 of 235

Title: Hardening networks against strategic attackers using attack graph games

Author(s): Durkota, K (Durkota, Karel); Lisy, V (Lisy, Viliam); Bosansky, B (Bosansky, Branislav); Kiekintveld, C (Kiekintveld, Chris (Pechoucek, Michal)

Source: COMPUTERS & SECURITY **Volume:** 87 **Article Number:** UNSP 101578 **DOI:** 10.1016/j.cose.2019.101578 **Published:** NO

Abstract: We consider the problem faced by a network administrator (defender) when deploying limited security resources to p strategic attacker. To evaluate the effectiveness of a defense strategy, one must consider possible counterattacks that an attack theory to model the interaction between the defender and the attacker. Game theory provides relevant concepts and algorithm strategies in environments with multiple decision makers. To model the space of attacker's possible actions, we use attack grap all known sequences of attacker's action that may lead to successful attack for a given network. We demonstrate our approach actions, where the defender deploys deceptive hosts and services (honeypots) to detect and mitigate attacks.

We assume the worst-case attacker who has a complete knowledge of the (typically randomized) defense strategy. We seek the against this attacker in the form of a Stackelberg equilibrium. Computing this solution exactly using standard techniques has lir investigate several approaches for increasing scalability to realistic problems. We introduce optimization methods for finding e and then propose a variety of polynomial heuristic algorithms that scale to significantly larger games. We analyze the scalabilit heuristic solutions on realistic network topologies. We show that the strategies found by the heuristics are often near-optimal a game-theoretic baselines. Finally, we show how attack graph games can be used to answer various research questions relevant administrators. (C) 2019 Elsevier Ltd. All rights reserved.

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Record 31 of 235

Title: A GPU solver for symmetric positive-definite matrices vs. traditional codes

Author(s): Bohacek, J (Bohacek, Jan); Kharicha, A (Kharicha, Abdellah); Ludwig, A (Ludwig, Andreas); Wu, MH (Wu, Menghuai); H Tobias); Karimi-Sibaki, E (Karimi-Sibaki, Ebrahim)

Source: COMPUTERS & MATHEMATICS WITH APPLICATIONS **Volume:** 78 **Issue:** 9 **Special Issue:** SI **Pages:** 2933-2943 **DOI:** 10.1016/j.camwa.2019.02.034 **Published:** NOV 1 2019

Abstract: In Heat Transfer and Fluid Flow Laboratory in Brno, the inverse heat conduction problem (IHCP) has been extensively boundary conditions at hot surfaces of solid materials cooled by spraying nozzles. More than three decades of experience and c has proven our experimental/numerical technique to be reliable and very accurate. However, a typical calculation requires rela The transient heat diffusion in a multi-material sample is the most computationally costly ingredient of the algorithm. In the pr speeding up our calculations is manifested by firstly benchmarking it against traditional CFD codes such as OpenFOAM (FDIC) a Secondly, we also unveil a unique comparison between the performance of three inhouse GPU codes each written by a differen Chronologically listed, one student pushed his luck with a fully explicit scheme, while the other two, including us, bet on implic by-line method in OpenCL and the conjugate gradient method with the deflated truncated Neumann series preconditioner in C

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Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Bohacek, Jan	C-2078-2018	0000-0003-3319-4254

ISSN: 0898-1221
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Record 32 of 235
Title: Engineering enzyme access tunnels
Author(s): Kokkonen, P (Kokkonen, Piia); Bednar, D (Bednar, David); Pinto, G (Pinto, Gaspar); Prokop, Z (Prokop, Zbynek); Damb
Source: BIOTECHNOLOGY ADVANCES **Volume:** 37 **Issue:** 6 **Article Number:** 107386 **DOI:** 10.1016/j.biotechadv.2019.04.008 **Pul**
Abstract: Enzymes are efficient and specific catalysts for many essential reactions in biotechnological and pharmaceutical indu natural enzymes do not display the catalytic efficiency, stability or specificity required for these industrial processes. The currer methods offer solutions to this problem, but they mainly target the buried active site where the chemical reaction takes place. I ignored, the tunnels and channels connecting the environment with the active site are equally important for the catalytic prope the enzymatic tunnels and channels affect enzyme activity, specificity, promiscuity, enantioselectivity and stability. This review emerging field of enzyme access tunnel engineering with case studies describing design of all the aforementioned properties. T analysis of geometry and function of the enzymatic tunnels and channels and for the rational design of tunnel modifications wi combination of new software tools and enzyme engineering strategies will provide enzymes with access tunnels and channels s individual industrial processes.
Accession Number: WOS:000484647000003
PubMed ID: 31026496
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Author	Web of Science ResearcherID	ORCID Number
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Damborsky, Jiri	H-3799-2012	0000-0002-7848-8216

ISSN: 0734-9750
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Record 33 of 235
Title: Molecular Dynamics of Graphene-Electrolyte Interface: Interfacial Solution Structure and Molecular Diffusion
Author(s): Dockal, J (Dockal, Jan); Moucka, F (Moucka, Filip); Lisal, M (Lisal, Martin)
Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 123 **Issue:** 43 **Pages:** 26379-26396 **DOI:** 10.1021/acs.jpcc.9b07487 **Pub**
Abstract: Graphene-based applications often take place in aqueous environments, and they benefit from a molecular-level und solutions in contact with graphene surfaces under different conditions. We study the aqueous solutions of electrolytes (LiCl, Na near the interface with a graphene sheet using classical molecular simulations. In order to model the graphene ion interactions effective polarizable model of Williams et al. (J. Phys. Chem. Lett. 2017, 8, 703). In order to thoroughly characterize the solution surface, in addition to standard structural properties, we employ our novel intermolecular bond definition based on the spatial provides numbers of water-water and water-ion intermolecular bonds per water molecule and number of water molecules per i distance from the graphene surface in a completely self-consistent manner. This thus allows summations of the bonds and qua bonds between different species in the solution. Our analysis shows that the interfacial structure exhibits a competition betwee formation of ion dense adsorption layers, and strong hydrogen and ion-water bonds in the solution; what is particularly interes compensation and the mutual symmetries of intermolecular bonding. Finally, we evaluate the lateral mobility of water and ion and bulk regions, showing significant reduction of the dynamics of both the water and the ions in the interfacial region compar
Accession Number: WOS:000493865700037
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Dockal, Jan		0000-0003-0551-0694

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Record 34 of 235

Title: From taxonomic deflation to newly detected cryptic species: Hidden diversity in a widespread African squeaker catfish

Author(s): Jirsova, D (Jirsova, Dagmar); Stefka, J (Stefka, Jan); Blazek, R (Blazek, Radim); Malala, JO (Malala, John O.); Lotuliak Mahmoud, ZN (Mahmoud, Zuheir N.); Jirku, M (Jirku, Miloslav)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 15748 **DOI:** 10.1038/s41598-019-52306-2 **Published:** OCT 31 2019

Abstract: Cryptic genetic diversity and erroneous morphological species determination represent frequent problems in biodive examination of 138 specimens of Synodontis (Mochokidae, Siluriformes) from the Nile River and Lake Turkana revealed the pre and S. frontosus-like morphotypes, with a phenotypic gradient between them. We concluded phylogenetic and population gen mitochondrial and one nuclear marker including 131 coxI (565 bp), 96 cytb (973 bp) and 19 RAG2 (896 bp) sequences from the N additional GenBank data of Synodontis spp. Whilst nuclear data were inconclusive, mitochondrial sequences suggested that bc intermediate forms are conspecific. The results imply probable synonymy of S. frontosus with S. schall. Conversely, a strong bic revealed among widely distributed and supposedly conspecific S. schall-like catfish of the Nilo-Sudanian ichthyological provinc stricto (=Eastern clade), as defined by type locality in the Nile, is apparently restricted to the eastern part of the Nilo-Sudanian i Nile, Turkana, Chad). Synodontis schall Western clade (Senegambia, Niger, Chad) most probably represents a cryptic taxon, unr absence of distinctive morphological differences.

Accession Number: WOS:000493439600046

PubMed ID: 31673053

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Stefka, Jan	N-3924-2019	0000-0002-1283-9730
Jirsova, Dagmar		0000-0002-1099-8076

ISSN: 2045-2322

Record 35 of 235

Title: Extreme nonassociativity in order nine and beyond

Author(s): Drapal, A (Drapal, Ales); Valent, V (Valent, Viliam)

Source: JOURNAL OF COMBINATORIAL DESIGNS **Volume:** 28 **Issue:** 1 **Pages:** 33-48 **DOI:** 10.1002/jcd.21679 **Early Access Date:** 2020

Abstract: The main concern of this paper are quasigroups of order nine that possess at most 18 associative triples. The order ni there exists a quasigroup (Q,*) such that x * (y * z)=(x * y) * z holds if and only if x=y=z. Up to isomorphism there is only one such has remarkable properties that bind it to a nearfield, to a PMD (9,4) and to a Sudoku division square.

Accession Number: WOS:000493296900001

ISSN: 1063-8539

eISSN: 1520-6610

Record 36 of 235

Title: Fast Screening of Inhibitor Binding/Unbinding Using Novel Software Tool CaverDock

Author(s): Pinto, GP (Pinto, Gaspar P.); Vavra, O (Vavra, Ondrej); Filipovic, J (Filipovic, Jiri); Stourac, J (Stourac, Jan); Bednar, D ((Damborsky, Jiri)

Source: FRONTIERS IN CHEMISTRY **Volume:** 7 **Article Number:** 709 **DOI:** 10.3389/fchem.2019.00709 **Published:** OCT 29 2019

Abstract: Protein tunnels and channels are attractive targets for drug design. Drug molecules that block the access of substrate efficient modulators of biological activity. Here, we demonstrate the applicability of a newly developed software tool CaverDoc drugs against pharmacologically relevant targets. First, we evaluated the effect of rigid and flexible side chains on sets of substr different proteins. In order to assess the accuracy of our software, we compared the results obtained from CaverDock calculatio previously collected with heat shock protein 90 alpha. Finally, we tested the virtual screening capabilities of CaverDock with a s inflammatory FDA-approved drugs with two molecular targets-cytochrome P450 17A1 and leukotriene A4 hydrolase/aminopep trajectories using four processors took on average 53 min per molecule with 90% successfully calculated cases. The screening ic based on the profile of potential energies of binding and unbinding trajectories. We concluded that CaverDock is a sufficiently f for screening binding/unbinding processes of pharmacologically important targets with buried functional sites. The standalone available freely at https://loschmidt.chemi.muni.cz/caverdock/and the web version at https://loschmidt.chemi.muni.cz/caverw

Accession Number: WOS:000497430300001

PubMed ID: 31737596

ISSN: 2296-2646

Record 37 of 235

Title: Experimental investigation of anode arc attachment area in DC arc plasma torch at low pressures

Author(s): Ondac, P (Ondac, P.); Maslani, A (Maslani, A.); Hrabovsky, M (Hrabovsky, M.)

Source: JOURNAL OF PHYSICS D-APPLIED PHYSICS **Volume:** 52 **Issue:** 40 **Article Number:** 405201 **DOI:** 10.1088/1361-6463/ab3

Abstract: The anode area and anode erosion of a DC arc plasma torch with an external anode are experimentally investigated u pressures, arc currents, and anode configurations. A high-speed camera, high-voltage probe, electric probes, and a Schlieren sy field in the anode area is measured using electric probes at arc electric currents lower than 100 A. It is found that a mean value the anode can be satisfactorily estimated in a non-intrusive way when the anode attachment is constricted. Anode erosion is pr can be compared in different experimental conditions just by quickly processing high-speed video footage, even while the plasr Anode erosion decreases along with ambient pressure and it is lower when a diffuse anode arc attachment is present as oppose attachment. The sources of plasma fluctuations inside and around the plasma jet are mainly the movement of the anode arc at vortices. The average speed of the anode arc attachment increases with decreases in ambient pressure. On the contrary, the av process, or the distance between the exit nozzle and the average attachment's position, decreases with reductions in ambient p pressure values for the transition between a constricted and diffuse anode arc attachment and for the transition between subs flow.

Accession Number: WOS:000478781600001

ISSN: 0022-3727

eISSN: 1361-6463

Record 38 of 235

Title: Transferrin Identification in Sterlet (Acipenser ruthenus) Reproductive System

Author(s): Xin, MM (Xin, Miaomiao); Vechtova, P (Vechtova, Pavlina); Shaliutina-Kolesova, A (Shaliutina-Kolesova, Anna); Fussy, (Loginov, Dmitry); Dzyuba, B (Dzyuba, Borys); Linhart, O (Linhart, Otomar); Boryshpolets, S (Boryshpolets, Serhii); Rodina, M (R Loginova, Y (Loginova, Yana); Sterba, J (Sterba, Jan)

Source: ANIMALS **Volume:** 9 **Issue:** 10 **DOI:** 10.3390/ani9100753 **Published:** OCT 2019

Abstract: Simple Summary Sturgeon is an ancient and unique fish species. Most of sturgeon are listed as critically endangered s alteration and overharvesting. Study of sturgeon reproductive system and sperm is important for aquaculture and conservatio recognized as a multiple task protein, positively correlated with spermatogenesis and sperm quality. Thus, we tried to detect tr out-of-spawning sterlet reproductive organs and sperm. Two transferrin genes, serotransferrin and melanotransferrin, have be organs of sterlet males. The serotransferrin was expressed higher in reproductive organs of spermiating than out-of-spawning s transferrin was detected in sterlet seminal plasma. This information contributes to the existing information on the variability of potential role of transferrin in chondrostean fishes.

Abstract Transferrins are a superfamily of iron-binding proteins and are recognized as multifunctional proteins. In the present s proteomic methods were used to identify transferrins in the reproductive organs and sperm of out-of-spawning and spermiatin males. The results showed that seven transferrin transcripts were identified in the transcriptome of sterlet, and these transcript different transferrin genes, serotransferrin and melanotransferrin, with several isoforms present for serotransferrin. The relative isoforms was higher in the kidneys and Wolffian ducts in the spermiating males compared to out-of-spawning males. In additio immunodetected in sterlet seminal plasma, but not in sterlet spermatozoa extract. Mass spectrometry identification of transfer in spermatozoa corroborates immunodetection. The identification of transferrin in the reproductive organs and seminal plasm provides the potential function of transferrin during sturgeon male reproduction.

Accession Number: WOS:000496757200050

PubMed ID: 31575042

ISSN: 2076-2615

Record 39 of 235

Title: Cohesive Properties of Ionic Liquids Calculated from First Principles

Author(s): Cervinka, C (Cervinka, Ctirad); Klajmon, M (Klajmon, Martin); Stejfa, V (Stejfa, Vojtech)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 15 **Issue:** 10 **Pages:** 5563-5578 **DOI:** 10.1021/acs.jctc.9b

Abstract: Low volatility of ionic liquids (ILs), being one of their most valuable properties, is also the principal factor making relia pressures and vaporization (or sublimation) enthalpies of ILs extremely difficult. Alternatively, vaporization enthalpies at the te can be obtained from the enthalpies of sublimation and fusion. While the latter can be obtained calorimetrically with a fair accu principle accessible through ab initio computations. This work assesses the performance of the first-principles calculations of s Namely, 3 compounds, coupling the 1-ethyl-3-methylimidazolium cation [emIm] with either tetrafluoroborate [BF4], hexafluorc bis(trifluoromethylsulfonyl)imide [NTf2] anions were selected for a case study. A computational methodology, originally develc adopted for crystals of ILs. It exploits periodic density functional theory (DFT) calculations of the unit-cell geometries and quasi many-body expansion schemes for ab initio refinements of the lattice energies of crystalline ILs. The vapor phase is treated as t

are obtained combining the rigid rotor-harmonic oscillator model with corrections from the one-dimensional hindered rotors a simulations capturing the contributions from the interionic interaction modes. Although the given computational approach ena chemical accuracy (4 kJ mol(-1)) of calculated sublimation enthalpies of simple molecular crystals, reaching the same level of a proves challenging as crystals of ionic liquids are bound appreciably stronger than common molecular crystals, the underlying ionic liquids is up to 1 order of magnitude larger. Still, combination of the mentioned computational and experimental framewo promising scheme that is expected to generate reliable and accurate temperature-dependent data on sublimation (and vaporiz

Accession Number: WOS:000489678700034

PubMed ID: 31436986

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Stejfa, Vojtech	G-9925-2018	0000-0002-2839-8546

ISSN: 1549-9618

eISSN: 1549-9626

Record 40 of 235

Title: Quantum Chemical Calculations of NMR Chemical Shifts in Phosphorylated Intrinsically Disordered Proteins

Author(s): Precechtelova, JP (Precechtelova, Jana Pavlikova); Mladek, A (Mladek, Arnost); Zapletal, V (Zapletal, Vojtech); Hritz, J

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 15 **Issue:** 10 **Pages:** 5642-5658 **DOI:** 10.1021/acs.jctc.8b

Abstract: Quantum mechanics (QM) calculations are applied to examine H-1, C-13, N-15, and P-31 chemical shifts of two phospl intrinsically disordered protein region. The QM calculations employ a combination of (1) structural ensembles generated by mo fragmentation technique based on the adjustable density matrix assembler, and (3) density functional methods. The combined used to obtain chemical shifts (i) in the S19 and S40 residues of the non-phosphorylated and (ii) in the pS19 and pS40 residues o human tyrosine hydroxylase 1 as the system of interest. We study the effects of conformational averaging and explicit solvent sa of phosphorylation on the computed chemical shifts. Good to great quantitative agreement with the experiment is achieved for systematic error cancellation is optimized by the choice of a suitable NMR standard. The effect of the standard reference on the chemical shifts is demonstrated by employing three different referencing methods. Error bars associated with the statistical ave chemical shifts are larger than the difference between the P-31 chemical shift of pS19 and pS40. The sequence trend of P-31 shif reliably reproduced. On the contrary, the calculations correctly predict the change of the C-13 chemical shift for CB induced by t serine residues. The present work demonstrates that QM calculations coupled with molecular dynamics simulations and fragm used as an alternative to empirical prediction tools in the structure characterization of intrinsically disordered proteins.

Accession Number: WOS:000489678700041

PubMed ID: 31487161

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Hritz, Jozef	J-6887-2015	0000-0002-4512-9241

ISSN: 1549-9618

eISSN: 1549-9626

Record 41 of 235

Title: Formation of CO+ by radiative association

Author(s): Zamecnikova, M (Zamecnikova, Martina); Soldan, P (Soldan, Pavel); Gustafsson, M (Gustafsson, Magnus); Nyman, G (

Source: MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY **Volume:** 489 **Issue:** 2 **Pages:** 2954-2960 **DOI:** 10.1093/mn 2019

Abstract: We theoretically estimate formation rate coefficients for CO+ through the radiative association of C+(P-2) with O(P-3). claimed radiative association to be the most important route for CO+ formation in SN 1987A. In 1990, Dalgarno, Du and You cha in this study, we improve previous estimates of the radiative association rate coefficients for forming CO+ from C+(P-2) and O(P- quantum mechanically based perturbation theory calculations as well as semiclassical calculations, which are combined with E add the effect of shape resonances. We explicitly include four electronic transitions. The required potential energy and transitic obtained through large basis set multireference configuration interaction electronic structure calculations. We report cross-sect obtain rate coefficients in the range of 10-10 000 K, finding that the CO+ formation rate coefficient is larger than the previous est our results support their claim that in SN 1987A, CO is mainly formed through radiative association and not through the charge CO + O+ as earlier suggested by Petuchowski et al.

Accession Number: WOS:000489298100109

Author Identifiers:

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Zamecnikova, Martina	H-3552-2014	0000-0003-1619-3583

ISSN: 0035-8711

eISSN: 1365-2966

Record 42 of 235

Title: Symbolic regression in dynamic scenarios with gradually changing targets

Author(s): Zegklitz, J (Zegklitz, Jan); Posik, P (Posik, Petr)

Source: APPLIED SOFT COMPUTING **Volume:** 83 **Article Number:** UNSP 105621 **DOI:** 10.1016/j.asoc.2019.105621 **Published:** C

Abstract: Symbolic regression is a machine learning task: given a training dataset with features and targets, find a symbolic fun target given the features. This paper concentrates on dynamic regression tasks, i.e. tasks where the goal changes during the mo is motivated by dynamic regression tasks originating in the domain of reinforcement learning: we study four dynamic symbolic to well-known reinforcement learning benchmarks, with data generated from the standard Value Iteration algorithm. We first sh the target function changes gradually, with no abrupt changes. Even these gradual changes, however, are a challenge to traditio based Symbolic Regression algorithms because they rely only on expression manipulation and selection. To address this challe enhancement to such algorithms suitable for dynamic scenarios with gradual changes, namely the recently introduced type of Combination of Features. This type of leaf node, aided by the error backpropagation technique known from artificial neural net to better fit the data by utilizing the error gradient to its advantage rather than searching blindly using only the fitness values. T baseline of the core algorithm without any of our improvements and also with a classic evolutionary dynamic optimization tech results show that the proposed modifications greatly improve the algorithm ability to track a gradually changing target. (C) 201 reserved.

Accession Number: WOS:000488100900015

ISSN: 1568-4946

eISSN: 1872-9681

Record 43 of 235

Title: Effect of high pressure on magnetic properties of CrMnFeCoNi high entropy alloy

Author(s): Kamarad, J (Kamarad, J.); Friak, M (Friak, M.); Kastil, J (Kastil, J.); Schneeweiss, O (Schneeweiss, O.); Sob, M (Sob, M.)

Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 487 **Article Number:** UNSP 165333 **DOI:** 10.1016/j.jmm OCT 1 2019

Abstract: The temperature and magnetic field dependences of magnetization of the Cantor CrMnFeCoNi alloy were studied at a external pressure. The low-temperature spin-glass-like behavior and the paramagnetic behavior at temperatures above 100 K w moment of the alloy, m(eff)= 2.71 mu(B)/f.u., were observed. A negative value of the paramagnetic Curie temperature, theta(c) confirms a presence of strong antiferromagnetic interactions of moments in the alloy. A model of the magnetic clusters with the 0.275 mu(B)/f.u. provides a possibility to describe qualitatively the pronounced difference between the pressure-induced decre ZFC and the FC alloys, dlnM/dP(5 K) = - 15.5*10(-3) GPa(-1) and - 39.2*10(-3) GPa(-1), respectively. The former value is in an excel value of - 16*10(-3) GPa(-1) obtained from our quantum-mechanical calculations. The negative pressure shift of the ordering ter dT(ord)/dP = - 9 K/GPa, and the pressure-induced decrease of magnetization of the alloy in paramagnetic state, dlnM/dP(90 K) = possible itinerant character of magnetism of the alloy. The results of theoretical calculations of the total moment of the CrMnFe

Accession Number: WOS:000471754300006

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kastil, Jiri	G-6719-2014	

ISSN: 0304-8853

eISSN: 1873-4766

Record 44 of 235

Title: Local atomic arrangement in LaCuAl3 and LaAuAl3 by NMR and density functional theory

Author(s): Chlan, V (Chlan, Vojtech); Dolezal, P (Dolezal, Petr); Sgallova, R (Sgallova, Rachel); Klicpera, M (Klicpera, Milan); Franz Javorsky, P (Javorsky, Pavel)

Source: JOURNAL OF PHYSICS-CONDENSED MATTER **Volume:** 31 **Issue:** 38 **Article Number:** 385601 **DOI:** 10.1088/1361-648X/a
2019

Abstract: CeCuAl3 and CeAuAl3, crystallizing in the non-centrosymmetric BaNiSn3 tetragonal structure, are known mainly for th
scattering spectra involving additional excitations ascribed to vibron quasi-bound quantum state in CeCuAl3 and anti-crossing
excitations in CeCuAl3. In this work, we present results of nuclear magnetic resonance (NMR) experiments on their lanthanum a
LaAuAl3. The character of NMR spectra of La-139, Al-27, and Cu-65 measured in LaAuAl3 and LaCuAl3 is dominated by electric q
spectral parameters acquired from experimental data are confronted with values obtained from the electronic structure calcula
remarkable differences for the two compounds. The La-139 spectrum in LaAuAl3 can be interpreted by a single spectral compor
uniform environment of La atoms in the crystal structure, whereas for LaCuAl3 the spectrum decomposition yields a wide distri
parameters, which is not possible to explain by a single La environment, and multiple non-equivalent La positions in the crystal
interpret the spectrum.

Accession Number: WOS:000473703900001

PubMed ID: 31170703

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Chlan, Vojtech	D-4868-2017	0000-0001-6963-9273

ISSN: 0953-8984

eISSN: 1361-648X

Record 45 of 235

Title: Revealing the metabolic capacity of Streblomastix strix and its bacterial symbionts using single-cell metagenomics

Author(s): Treitli, SC (Treitli, Sebastian C.); Kolisko, M (Kolisko, Martin); Husnik, F (Husnik, Filip); Keeling, PJ (Keeling, Patrick J.);

Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA **Volume:** 116 **Issue:** 39
10.1073/pnas.1910793116 **Published:** SEP 24 2019

Abstract: Lower termites harbor in their hindgut complex microbial communities that are involved in the digestion of cellulose.
which are usually associated with specific bacterial symbionts found on their surface or inside their cells. While these form the f
system in symbiosis research, we still know little about the functional basis for most of these relationships. Here, we describe th
relationship between one protist, the oxymonad Streblomastix strix, and its ectosymbiotic bacterial community using single-ce
partial assemblies of the host S. strix genome and Candidatus Ordinivivax streblomastigis, as well as a complex metagenome as
Bacteroidetes bacteria confirmed by ribosomal (r)RNA fluorescence in situ hybridization (FISH) to be associated with S. strix. Ou
probably not involved in the cellulose digestion, but the bacterial community on its surface secretes a complex array of glycosyl
with the ability to degrade cellulose to monomers and fueling the metabolism of S. strix. In addition, some of the bacteria can fi
theoretically provide S. strix with essential amino acids and cofactors, which the protist cannot synthesize. On the contrary, mo
lack the essential glycolytic enzyme enolase, which may be overcome by the exchange of intermediates with S. strix. This study
the combined single-cell (meta)genomic and FISH approach for studies of complicated symbiotic systems.

Accession Number: WOS:000487532900068

PubMed ID: 31492817

ISSN: 0027-8424

Record 46 of 235

Title: Chemistry of 2,14-Dithiacalix[4]arene: Alkylation and Conformational Behavior of Peralkylated Products

Author(s): Kortus, D (Kortus, Daniel); Miksatko, J (Miksatko, Jiri); Kundrat, O (Kundrat, Ondrej); Babor, M (Babor, Martin); Eigner,
H (Dvorakova, Hana); Lhotak, P (Lhotak, Pavel)

Source: JOURNAL OF ORGANIC CHEMISTRY **Volume:** 84 **Issue:** 18 **Pages:** 11572-11580 **DOI:** 10.1021/acs.joc.9b01493 **Publishe**

Abstract: 2,14-Dithiacalix[4]arene, prepared on a multigram scale, was alkylated using the reaction conditions well known from
calixarenes or thiacalixarenes to study the specific conformational preferences and dynamic behavior of the corresponding tetr
proved by the combination of the X-ray crystallography and dynamic NMR techniques, the presence of mixed bridges (-CH2- an
skeleton brings about considerable changes in the mutual ratios of the individual conformers compared to the parent macrocy
conformers, hardly accessible for common calixarenes/thiacalixarenes (e.g., 1,2-alternates) are easily prepared in very good yie
dithiacalix[4]arene, which makes this mixed-bridge system attractive as molecular scaffold for supramolecular applications.

Accession Number: WOS:000487576900019

PubMed ID: 31438675

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Babor, Martin		0000-0002-0268-4640

ISSN: 0022-3263

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Record 47 of 235

Title: Oxidation potentials of guanine, guanosine and guanosine-5 '-monophosphate: Theory and experiment

Author(s): Liska, A (Liska, Alan); Triskova, I (Triskova, Iveta); Ludvik, J (Ludvik, Jiri); Trnkova, L (Trnkova, Libuse)

Source: ELECTROCHIMICA ACTA **Volume:** 318 **Pages:** 108-119 **DOI:** 10.1016/j.electacta.2019.06.052 **Published:** SEP 20 2019

Abstract: Guanine, having lower one-electron oxidation potential than other nucleobases, is of relevance to oxidative degradati mutagenesis, carcinogenesis, and aging. Here we compare oxidation potentials of guanine (G), guanosine (Guo), deoxyguanosi monophosphate (GMP) and 2'-deoxyguanosine-5'-monophosphate (dGMP) obtained by theoretical and experimental methods optimized and the identities of minima were verified by vibration frequency calculations. Redox equilibria were modelled in ter thermochemical cycles. The changes in free energy were calculated at DFT level using the two different functionals: (i) general p (ii) more specific omega B97X-D functional (both with 6-31 + G(d) basis set). Experimental oxidation potentials of all G analogue metrically on a polymer pencil graphite electrode (pPeGE) providing the best results from all carbon electrodes used (glassy ca edge plane pyrolytic graphite electrodes). The oxidation process is strongly dependent on the pH value and with increasing pH peaks (E-pa) towards negative potentials is observed. The theoretically and experimentally obtained oxidation potentials were Anodic peak potentials increase in the order G << dGMP <= GMP < dGuo <= Guo and correlate with the calculated thermodynam with NBO charges in purine moiety. The oxidation of deoxy analogues was predicted theoretically to occur at lower potentials t parent compounds and this fact was experimentally verified. The assumption that due to negatively charged phosphate group oxidation potentials could be observed at lower positive potential has not been confirmed and the significant difference (more oxidation potentials of G nucleobase and its nucleosides and nucleotides is discussed. Moreover, conformity of theoretical and (cation, neutral) indicates that while the deprotonation process of G differs from its analogues, the oxidation process of all spec ring. (C) 2019 Published by Elsevier Ltd.

Accession Number: WOS:000478969600013

ISSN: 0013-4686

eISSN: 1873-3859

Record 48 of 235

Title: Solution to the Balitsky-Kovchegov equation with the collinearly improved kernel including impact-parameter dependen

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

Source: PHYSICAL REVIEW D **Volume:** 100 **Issue:** 5 **Article Number:** 054015 **DOI:** 10.1103/PhysRevD.100.054015 **Published:** SE

Abstract: The solution to the impact-parameter dependent Balitsky-Kovchegov equation with the collinearly improved kernel i solution does not present the phenomenon of Coulomb tails at large impact parameters that have affected previous studies. Th explored numerically. It is found to be linked to the fact that this kernel suppresses large daughter dipoles. Solutions based on the initial condition are used to compute predictions for structure functions of the proton and the exclusive photoproduction a vector mesons. A reasonable agreement is found when comparing to HERA and LHC data.

Accession Number: WOS:000486642100004

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 2470-0010

eISSN: 2470-0029

Record 49 of 235

Title: Bifurcated hydrogen bonds in platinum(II) complexes with phosphinoamine ligands

Author(s): Sojka, M (Sojka, Martin); Tousek, J (Tousek, Jaromir); Badri, Z (Badri, Zahra); Foroutan-Nejad, C (Foroutan-Nejad, Cin

Source: POLYHEDRON **Volume:** 170 **Pages:** 593-601 **DOI:** 10.1016/j.poly.2019.06.014 **Published:** SEP 15 2019

Abstract: In this work we report an investigation of the influence of bifurcated intramolecular hydrogen bonds on conformatio with phosphinoamine ligands. The series of new cis and trans-PtCl2L2 complexes with phosphinoamine ligands was synthesize P-31, Pt-195 NMR, IR, and molecular structures of 8 complexes were determined by X-ray crystallography. The hydrogen bonds center dot center dot center dot CIPt and NH center dot center dot center dot R (R = COOCH3, C(O)CH3, F, CN) moieties of the lig

structural data from X-ray diffraction are linked to calculated conformational energies from density functional theory (DFT) and obtained from quantum theory of atoms in molecules (QTAIM) calculations. The most prominent NH center dot center dot cent found in the cis complexes with para substituted phosphinoamine ligands, which show delocalization indexes (DI) up to 0.09. Tl phosphinoamine ligands decrease the DI values down to zero for C(O)OCH3 and C(O)CH3 moieties. (C) 2019 Elsevier Ltd. All rigl

Accession Number: WOS:000489192100068

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sojka, Martin		0000-0001-5266-3963
Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173

ISSN: 0277-5387

Record 50 of 235

Title: Transfer and Amplification of Chirality Within the "Ring of Fire" Observed in Resonance Raman Optical Activity Experimen

Author(s): Li, GJ (Li, Guojie); Kessler, J (Kessler, Jiri); Cheramy, J (Cheramy, Joseph); Wu, T (Wu, Tao); Poopari, MR (Poopari, Mol Petr); Xu, YJ (Xu, Yunjie)

Source: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 58 **Issue:** 46 **Pages:** 16495-16498 **DOI:** 10.1002/anie.201909 2019 **Published:** NOV 11 2019

Abstract: We report extremely strong chirality transfer from a chiral nickel complex to solvent molecules detected as Raman op energies of the complex were in resonance with the excitation-laser light. The phenomenon was observed for a wide range of a chiral 2-butanol, the induced ROA was even stronger than the natural one. The observations were related to so-called quantum enable a strong chiral Rayleigh scattering of the resonating complex. According to a model presented here, the maximal induce certain distance from the solute, in a three-dimensional "ring of fire", even after rotational averaging. Most experimental ROA si could be reproduced. The effect might significantly increase the potential of ROA spectroscopy in bioimaging and sensitive dete

Accession Number: WOS:000486398200001

PubMed ID: 31460686

Author Identifiers:

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Xu, Yunjie	G-6542-2014	0000-0003-3736-3190

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Page 2 (Records 51 -- 100)
[1 | 2 | 3 | 4 | 5]

Record 51 of 235

Title: Nanomotor tracking experiments at the edge of reproducibility

Author(s): Novotny, F (Novotny, Filip); Pumera, M (Pumera, Martin)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 13222 **DOI:** 10.1038/s41598-019-49527-w **Published:** SEP 13 2019

Abstract: The emerging field of self-propelling micro/nanorobots is teeming with a wide variety of novel micro/ nanostructures self-propulsion in a liquid environment. As the size of these microscopic movers diminishes into the fully nanosized region, the micromotor become a random walk of colloidal particles. To test such colloidal samples for self-propulsion, the commonly ado to the mean squared displacement (MSD) function of the measured particle tracks. The practical significance of the result stron collected particle data and the sampling rate of the particle track. Because micro/nanomotor preparation methods are mostly l experimental data in published results is often on the edge of reproducibility. To address the situation, we perform MSD analysi as simulated dataset. These data are used to explore the effects of MSD analysis on limited data and several situations where th insignificant results.

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PubMed ID: 31519985

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ISSN: 2045-2322

Record 52 of 235

Title: Real-space dynamical mean-field theory of Friedel oscillations in strongly correlated electron systems

Author(s): Chatterjee, B (Chatterjee, B.); Skolimowski, J (Skolimowski, J.); Makuch, K (Makuch, K.); Byczuk, K (Byczuk, K.)

Source: PHYSICAL REVIEW B **Volume:** 100 **Issue:** 11 **Article Number:** 115118 **DOI:** 10.1103/PhysRevB.100.115118 **Published:** S

Abstract: We study Friedel oscillations and screening effects of the impurity potential in the Hubbard model. Electronic correlat solving the real-space dynamical mean-field theory equations using the continuous-time quantum Monte Carlo simulations at f a homogeneous self-energy approximation with the numerical renormalization group at zero temperature. We find that in the F amplitudes of Friedel oscillations and the screening charge decrease with increasing the interaction and follow the behavior of renormalization factor. Inside the Mott insulator regime, the Friedel oscillations are absent but the residual screening charge re

Accession Number: WOS:000485192700003

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ISSN: 2469-9950

eISSN: 2469-9969

Record 53 of 235

Title: Force Field Comparison of GM1 in a DOPC Bilayer Validated with AFM and FRET Experiments

Author(s): Owen, MC (Owen, Michael C.); Karner, A (Karner, Andreas); Sachl, R (Sachl, Radek); Preiner, J (Preiner, Johannes); Am Vacha, R (Vacha, Robert)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 123 **Issue:** 35 **Special Issue:** SI **Pages:** 7504-7517 **DOI:** 10.1021/acs.jpcl 2019

Abstract: The great physiological relevance of glycolipids is being increasingly recognized, and glycolipid interactions have bee cell recognition, neuronal plasticity, protein-ligand recognition, and other important processes. However, detailed molecular-le processes remains to be fully resolved. Molecular dynamics simulations could reveal the details of the glycolipid interactions, b influenced by the choice of the employed force field. Here, we have compared the behavior and properties of GM1, a common, l glycolipid, using the CHARMM36, OPLS, GROMOS, and Amber99-GLYCAMO6 (in bilayers comprising SLIPIDS and LIPID14 lipids) f comprising 1,2-dioleoyl-snglycero-3-phosphocholine lipids and compared the results to atomic force microscopy and fluoresce transfer experiments. We found discrepancies within the GM1 behavior displayed between the investigated force fields. Based c

complementary experimental results derived from fluorescence and AFM measurements, we recommend using the Amber99-G comprising LIPID14 or SLIPIDS lipids followed by CHARMM36 and OPLS force fields in simulations. The GROMOS force field is nc reproducing the properties of the GM1 head group.

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PubMed ID: 31397569

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ISSN: 1520-6106

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Record 54 of 235

Title: Concurrent Compression of Phospholipid Membranes by Calcium and Cholesterol

Author(s): Melcrova, A (Melcrova, Adela); Pokorna, S (Pokorna, Sarka); Vosahlikova, M (Vosahlikova, Miroslava); Sykora, J (Sykor Petr); Hof, M (Hof, Martin); Cwiklik, L (Cwiklik, Lukasz); Jurkiewicz, P (Jurkiewicz, Piotr)

Source: LANGMUIR **Volume:** 35 **Issue:** 35 **Pages:** 11358-11368 **DOI:** 10.1021/acs.langmuir.9b00477 **Published:** SEP 3 2019

Abstract: Regulation of cell metabolism, membrane fusion, association of proteins with cellular membranes, and cellular signal possible without Ca2+ ions. The distribution of calcium within the cell is uneven with the negatively charged inner leaflet of the of the primary targets of its accumulation. Therefore, we decided to map the influence of Ca2+ on the properties of lipid bilayer lipid membranes. We combined fluorescence spectroscopy (analysis of time-resolved emission spectra of Laurdan probe and d relaxation time related to local lipid mobility, and total emission shift reflecting membrane polarity and hydration) with molecu determine the effect of the increasing CaCl2 concentration on model lipid membranes containing POPC, POPS, and cholesterol calcium on the plasma membranes isolated from HEK293 cells was investigated using the steady-state fluorescence of Laurdan increases rigidity of all the model lipid membranes used, elevates their thickness, increases lipid packing and ordering, and imp All these effects were to a great extent similar to those elicited by cholesterol. However, the changes of the membrane propertie cholesterol seem largely independent from each other. At sufficiently high concentrations of calcium or cholesterol, the steric e alteration of membrane organization, i.e., the compressibility limit of membrane structures was reached. We found no indicatic between Ca2+ and cholesterol, nor competition of Ca2+ ions and hydroxyl groups of cholesterol for binding to phospholipids. F indicated that Ca2+ adsorption decreases mobility within the carbonyl region of model bilayers more efficiently than monovale > K+ > Cs+). The effects of calcium ions were to a great extent mitigated in the plasma membranes isolated from HEK293 cells w lipid membranes. Noticeably, the plasma membranes showed remarkably higher resistance toward rigidification induced by ca compared with the model membranes containing cholesterol.

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PubMed ID: 31393734

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Melcrova, Adela	F-6604-2014	0000-0001-6390-0522
Sykora, Jan	F-5179-2014	

ISSN: 0743-7463

Record 55 of 235

Title: Calculations of the relative populations of Lu@C-82 isomers

Author(s): Slanina, Z (Slanina, Zdenek); Uhlik, F (Uhlik, Filip); Shen, WQ (Shen, Wangqiang); Akasaka, T (Akasaka, Takeshi); Lu, X (Adamowicz, Ludwik)

Source: FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES **Volume:** 27 **Issue:** 9 **Pages:** 710-714 **DOI:** 10.1080/15363 SEP 2 2019

Abstract: Relative populations of five IPR (isolated-pentagon-rule) isomers of Lu@C-82 are computed using the Gibbs energy ba density functional theory calculations (B3LYP/6-31G*-SDD entropy term, B2PLYPD/6-31G*-SDD energetics). In agreement with o has the C-2v;9 cage.

Accession Number: WOS:000484156700007

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ISSN: 1536-383X

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Record 56 of 235

Title: CDK12 controls G1/S progression by regulating RNAPII processivity at core DNA replication genes

Author(s): Manavalan, APC (Manavalan, Anil Paul Chirackal); Pilarova, K (Pilarova, Kveta); Kluge, M (Kluge, Michael); Bartholome Koen); Rajecky, M (Rajecky, Michal); Oppelt, J (Oppelt, Jan); Khirsariya, P (Khirsariya, Prashant); Paruch, K (Paruch, Kamil); Krejc (Friedel, Caroline C.); Blazek, D (Blazek, Dalibor)

Source: EMBO REPORTS **Volume:** 20 **Issue:** 9 **Article Number:** e47592 **Published:** SEP 2019

Abstract: CDK12 is a kinase associated with elongating RNA polymerase II (RNAPII) and is frequently mutated in cancer. CDK12 c expression of homologous recombination (HR) DNA repair genes, but comprehensive insight into its target genes and cellular p chemical genetic approach to inhibit analog-sensitive CDK12, and find that CDK12 kinase activity is required for transcription o and thus for G1/S progression. RNA-seq and ChIP-seq reveal that CDK12 inhibition triggers an RNAPII processivity defect charac reads from 3 ' ends of predominantly long, poly(A)-signal-rich genes. CDK12 inhibition does not globally reduce levels of RNAPI However, individual CDK12-dependent genes show a shift of P-Ser2 peaks into the gene body approximately to the positions wh transcription were lost. Thus, CDK12 catalytic activity represents a novel link between regulation of transcription and cell cycle DNA replication and HR DNA repair defects as a consequence of CDK12 inactivation underlie the genome instability phenotype

Accession Number: WOS:000486091900003

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eISSN: 1469-3178

Record 57 of 235

Title: Next-generation sequencing of immunoglobulin gene rearrangements for clonality assessment: a technical feasibility stu

Author(s): Scheijen, B (Scheijen, Blanca); Meijers, RWJ (Meijers, Ruud W. J.); Rijntjes, J (Rijntjes, Jos); van der Klift, MY (van der K (Moebs, Markus); Steinhilber, J (Steinhilber, Julia); Reigl, T (Reigl, Tomas); van den Brand, M (van den Brand, Michiel); Kotrova, M JM (Ritter, Julia-Marie); Catherwood, MA (Catherwood, Mark A.); Stamatopoulos, K (Stamatopoulos, Kostas); Bruggemann, M (B (Davi, Frederic); Darzentas, N (Darzentas, Nikos); Pott, C (Pott, Christiane); Fend, F (Fend, Falko); Hummel, M (Hummel, Michael) Anton W.); Groenen, PJTA (Groenen, Patricia J. T. A.)

Group Author(s): EuroClonality-NGS Working Grp

Source: LEUKEMIA **Volume:** 33 **Issue:** 9 **Pages:** 2227-2240 **DOI:** 10.1038/s41375-019-0508-7 **Published:** SEP 2019

Abstract: One of the hallmarks of B lymphoid malignancies is a B cell clone characterized by a unique footprint of clonal immur rearrangements that serves as a diagnostic marker for clonality assessment. The EuroClonality/BIOMED-2 assay is currently the IG heavy chain (IGH) and x light chain (IGK) gene rearrangements of suspected B cell lymphomas. Here, the EuroClonality-NGS W multicentre technical feasibility study of a novel approach involving next-generation sequencing (NGS) of IGH and IGK loci rearr suitable for detecting IG gene rearrangements in frozen and formalin-fixed paraffin-embedded tissue specimens. By employing and IGK amplifying smaller amplicon sizes in combination with deep sequencing technology, this NGS -based IG clonality analy performance, even in DNA samples of suboptimal DNA integrity, and a high clinical sensitivity for the detection of clonal rearrar analyses of the high-throughput sequencing data with ARResT/Interrogate, a platform developed within the EuroClonality-NGS accurate identification of clonotypes in both polyclonal cell populations and monoclonal lymphoproliferative disorders. This m an important step towards implementation of NGS -based clonality assessment in clinical practice, which will eventually impro

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PubMed ID: 31197258

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Record 58 of 235

Title: Standardized next-generation sequencing of immunoglobulin and T-cell receptor gene recombinations for MRD marker id lymphoblastic leukaemia; a EuroClonality-NGS validation study

Author(s): Bruggemann, M (Brueggemann, Monika); Kotrova, M (Kotrova, Michaela); Knecht, H (Knecht, Henrik); Bartram, J (Bar (Boudjogrha, Myriam); Bystry, V (Bystry, Vojtech); Fazio, G (Fazio, Grazia); Fronkova, E (Fronkova, Eva); Giraud, M (Giraud, Mathie Hancock, J (Hancock, Jeremy); Herrmann, D (Herrmann, Dietrich); Jimenez, C (Jimenez, Cristina); Krejci, A (Krejci, Adam); Mopp T (Reigl, Tomas); Salson, M (Salson, Mikael); Scheijen, B (Scheijen, Blanca); Schwarz, M (Schwarz, Martin); Songia, S (Songia, Sin Michael); van Dongen, JJM (van Dongen, Jacques J. M.); Villarese, P (Villarese, Patrick); Wakeman, S (Wakeman, Stephanie); Wrig Cazzaniga, G (Cazzaniga, Giovanni); Davi, F (Davi, Frederic); Garcia-Sanz, R (Garcia-Sanz, Ramon); Gonzalez, D (Gonzalez, David) Patricia J. T. A.); Hummel, M (Hummel, Michael); Macintyre, EA (Macintyre, Elizabeth A.); Stamatopoulos, K (Stamatopoulos, Kos Trka, J (Trka, Jan); Darzentas, N (Darzentas, Nikos); Langerak, AW (Langerak, Anton W.)

Group Author(s): EuroClonality-NGS Working Grp

Source: LEUKEMIA **Volume:** 33 **Issue:** 9 **Pages:** 2241-2253 **DOI:** 10.1038/s41375-019-0496-7 **Published:** SEP 2019

Abstract: Amplicon-based next-generation sequencing (NGS) of immunoglobulin (IG) and T-cell receptor (TR) gene rearrangeme marker identification and quantification of minimal residual disease (MRD) in lymphoid neoplasms has been the focus of intens application. However, standardization and validation in a scientifically controlled multicentre setting is still lacking. Therefore, design, including bioinformatics, was performed within the EuroClonality-NGS working group and validated for MRD marker ide lymphoblastic leukaemia (ALL). Five EuroMRD ALL reference laboratories performed IG/TR NGS in 50 diagnostic ALL samples, a those generated through routine IG/TR Sanger sequencing. A central polytarget quality control (cPT-QC) was used to monitor pr central in-tube quality control (cIT-QC) was spiked into each sample as a library-specific quality control and calibrator. NGS ider 5.2/sample, range 0-14) clonal sequences vs. Sanger-sequencing 248 (average 5.0/sample, range 0-14). NGS primers covered po types more completely compared with local multiplex PCR sets and enabled sequencing of bi-allelic rearrangements and weak showed high reproducibility across all laboratories. These validated and reproducible quality-controlled EuroClonality-NGS ass standardized NGS-based identification of IG/TR markers in lymphoid malignancies.

Accession Number: WOS:000484399300009
PubMed ID: 31243313

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Record 59 of 235

Title: Quality control and quantification in IG/TR next-generation sequencing marker identification: protocols and bioinformati EuroClonality-NGS

Author(s): Knecht, H (Knecht, Henrik); Reigl, T (Reigl, Tomas); Kotrova, M (Kotrova, Michaela); Appelt, F (Appelt, Franziska); Stev V (Bystry, Vojtech); Krejci, A (Krejci, Adam); Grioni, A (Grioni, Andrea); Pal, K (Pal, Karol); Stranska, K (Stranska, Kamila); Plevova, (Rijntjes, Jos); Songia, S (Songia, Simona); Svaton, M (Svaton, Michael); Fronkova, E (Fronkova, Eva); Bartram, J (Bartram, Jack); Blanca); Herrmann, D (Herrmann, Dietrich); Garcia-Sanz, R (Garcia-Sanz, Ramon); Hancock, J (Hancock, Jeremy); Moppett, J (M JJM (van Dongen, Jacques J. M.); Cazzaniga, G (Cazzaniga, Giovanni); Davi, F (Davi, Frederic); Groenen, PJTA (Groenen, Patricia J Michael); Macintyre, EA (Macintyre, Elizabeth A.); Stamatopoulos, K (Stamatopoulos, Kostas); Trka, J (Trka, Jan); Langerak, AW (Gonzalez, D (Gonzalez, David); Pott, C (Pott, Christiane); Bruggemann, M (Brueggemann, Monika); Darzentas, N (Darzentas, Niko

Group Author(s): EuroClonality-NGS Working Grp

Source: LEUKEMIA **Volume:** 33 **Issue:** 9 **Pages:** 2254-2265 **DOI:** 10.1038/s41375-019-0499-4 **Published:** SEP 2019

Abstract: Assessment of clonality, marker identification and measurement of minimal residual disease (MRD) of immunoglobul gene rearrangements in lymphoid neoplasms using next-generation sequencing (NGS) is currently under intensive developmen diagnostics. So far, however, there is a lack of suitable quality control (QC) options with regard to standardisation and quality m clinical application of such approaches. The EuroClonality-NGS Working Group has therefore established two types of QCs to ac

IG/TR assays. First, a central polytarget QC (cPT-QC) is used to monitor the primer performance of each of the EuroClonality mu standardised human cell line-based DNA control is spiked into each patient DNA sample to work as a central in-tube QC and cal (cIT-QC). Having integrated those two reference standards in the ARResT/Interrogate bioinformatic platform, EuroClonality-NGS for standardised IG/TR gene rearrangement analysis by NGS with high reproducibility, accuracy and precision for valid marker i quantification in diagnostics of lymphoid malignancies.

Accession Number: WOS:000484399300010

PubMed ID: 31227779

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Garcia-Sanz, Ramon	B-7986-2017	0000-0003-4120-2787

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Record 60 of 235

Title: Inferential procedures for partially observed functional data

Author(s): Kraus, D (Kraus, David)

Source: JOURNAL OF MULTIVARIATE ANALYSIS **Volume:** 173 **Pages:** 583-603 **DOI:** 10.1016/j.jmva.2019.05.002 **Published:** SEP 2

Abstract: In functional data analysis it is usually assumed that all functions are completely, densely or sparsely observed on the applications have brought attention to situations where each functional variable may be observed only on a subset of the dom about the function is available on the complement. Various advanced methods for such partially observed functional data have interestingly, some essential methods, such as K-sample tests of equal means or covariances and confidence intervals for eigen are lacking. Without requiring any complete curves in the data, we derive asymptotic distributions of estimators of the mean fu and eigenelements and construct hypothesis tests and confidence intervals. To overcome practical difficulties with storing large memory, which arise due to partial observation, we use the nonparametric bootstrap approach. The proposed methods are inv simulations and on a fragmentary functional data set from medical research. (C) 2019 Elsevier Inc. All rights reserved.

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Record 61 of 235

Title: Coherent and incoherent vector meson electroproduction in the future electron - ion colliders: The hot - spot predictions

Author(s): Krelina, M (Krelina, M.); Goncalves, VP (Goncalves, V. P.); Cepila, J (Cepila, J.)

Source: NUCLEAR PHYSICS A **Volume:** 989 **Pages:** 187-200 **DOI:** 10.1016/j.nuclphysa.2019.06.009 **Published:** SEP 2019

Abstract: One of the more promising observables to probe the high energy regime of the QCD dynamics in the future Electron - exclusive vector meson production cross section in coherent and incoherent interactions. Such processes measure the average in the target as well the fluctuations and correlations in the gluon density. In this paper we present a comprehensive analysis of atomic number and momentum transfer dependencies of the coherent and incoherent cross sections considering two different profile function. In particular, we present the predictions of the hot - spot model, which assumes the presence of subnucleonic energy-dependent profile. Our results indicate that the analysis of the ratio between the incoherent and coherent cross section distributions in the future EIC can be useful to constrain the description of the hadronic structure at high energies. (C) 2019 Else

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Record 62 of 235

Title: Transcription of specific auxin efflux and influx carriers drives auxin homeostasis in tobacco cells

Author(s): Muller, K (Muller, Karel); Hosek, P (Hosek, Petr); Lankova, M (Lankova, Martina); Vosolsobe, S (Vosolsobe, Stanislav); M Katerina); Carna, M (Carna, Maria); Filova, M (Filova, Marketa); Dobrev, PI (Dobrev, Petre, I); Helusova, M (Helusova, Michaela); H Petrasek, J (Petrasek, Jan)

Source: PLANT JOURNAL **Volume:** 100 **Issue:** 3 **Pages:** 627-640 **DOI:** 10.1111/tpj.14474 **Early Access Date:** AUG 2019 **Publishe**

Abstract: Auxin concentration gradients are informative for the transduction of many developmental cues, triggering downstre responses. The generation of auxin gradients depends significantly on cell-to-cell auxin transport, which is supported by the ac influx carriers. However, at the level of individual plant cell, the co-ordination of auxin efflux and influx largely remains unchara issue by analyzing the contribution of canonical PIN-FORMED (PIN) proteins to the carrier-mediated auxin efflux in Nicotiana tal (BY-2) tobacco cells. We show here that a majority of canonical NtPINs are transcribed in cultured cells and in planta. Cloning of inducible overexpression in tobacco cells uncovered high auxin efflux activity of NtPIN11, accompanied by auxin starvation sym parameters after NtPIN11 overexpression were further assessed using radiolabelled auxin accumulation and mathematical mo experiments showed notable stimulation of auxin influx, which was accompanied by enhanced transcript levels of genes for a s by decreased transcript levels of other genes for auxin efflux carriers. A similar transcriptional response was observed upon rem medium, which resulted in decreased auxin efflux. Overall, our results revealed an auxin transport-based homeostatic mechani endogenous auxin levels. Open Research Badges This article has earned an Open Data Badge for making publicly available the necessary to reproduce the reported results. The data is available at

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PubMed ID: 31349380

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Record 63 of 235

Title: Coordination chemistry of 2D and layered gray arsenic: photochemical functionalization with chromium hexacarbonyl

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

Source: NPG ASIA MATERIALS **Volume:** 11 **Article Number:** 42 **DOI:** 10.1038/s41427-019-0142-x **Published:** AUG 23 2019

Abstract: The functionalization of layered materials is one of the current challenges in material science. Exfoliated rhombohedr promising layered material for the fabrication of electronic devices and sensors; however, synthetic protocols for tuning its pro surface by covalent functionalization are not known. In this communication, we present its covalent functionalization accompa rhombohedral arsenic in the presence of ultraviolet light irradiation and chromium hexacarbonyl. During this modification, the to the chromium metal center. We believe that this study provides a promising approach for the modification of rhombohedral enables its application in various fields, including electronic devices, sensors, and energy devices.

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Author Identifiers:

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Record 64 of 235

Title: Physical nature of silaneMIDLINE HORIZONTAL ELLIPSIScarbene dimers revealed by state-of-the-art ab initio calculations

Author(s): Yourdkhani, S (Yourdkhani, Sirous); Jablonski, M (Jablonski, Miroslaw)

Source: JOURNAL OF COMPUTATIONAL CHEMISTRY **Volume:** 40 **Issue:** 30 **Pages:** 2643-2652 **DOI:** 10.1002/jcc.26043 **Early Acc Published:** NOV 15 2019

Abstract: Using the SAPT2 + 3(CCD)delta MP2 method in complete basis set (CBS) limit, it is shown that the interactions in the re HORIZONTAL ELLIPSIScarbene dimers are mainly dispersive in nature. Consequently, slow convergence of dispersion energy al the interaction energy. Therefore, obtaining very accurate values requires extrapolation of the correlation part to the CBS limit. obtained at the CCSD(T)/CBS level of theory show that the studied silaneMIDLINE HORIZONTAL ELLIPSIScarbene dimers are rat

interaction energies ranging from about -1.9 to -1.3 kcal/mol. Comparing to CCSD(T)/CBS, it will be shown that SCS-MP2 and MP underestimate and methods based on SAPT2+ and having some third-order corrections, as well as the MP2 method, overestima energies. Popular SAPT(DFT) method performs better than SCS-MP2 and MP2C; nevertheless, underestimation is still considera slightly quenched if third-order dispersion energy and its exchange counterpart is added to the SAPT(DFT). The closest value of by the SAPT2 + (3)(CCD)delta MP2 method in quadruple-zeta basis set. (c) 2019 Wiley Periodicals, Inc.

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Author Identifiers:

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Record 65 of 235

Title: Proton Transfer Reactions between Methanol and Formic Acid Deposited on Free Ar-N Nanoparticles

Author(s): Pysanenko, A (Pysanenko, Andriy); Gamez, F (Gamez, Francisco); Farnikova, K (Farnikova, Karolina); Pluharova, E (Plu (Farnik, Michal)

Source: JOURNAL OF PHYSICAL CHEMISTRY A **Volume:** 123 **Issue:** 33 **Pages:** 7201-7209 **DOI:** 10.1021/acs.jpca.9b05372 **Publis**

Abstract: We have sequentially picked up two astrochemically relevant Bronsted acids (methanol and formic acid) on the surfa acting as a cold support. Photoionization and electron ionization yield (HCOOH)(x)H+, (CH3OH)(x)H+, and mixed protonated clu perdeuterated methanol CD3OD demonstrate notable proton transfer (PT) to formic acid acting as a proton acceptor in additior which is, perhaps, a more intuitive one. We, therefore, for the first time observed reactions between two different complex mole on argon nanoparticles. The experimental results are compared with state-of-the-art quantum chemistry calculations, showing and HCOOH center dot+ radical cations resulting from ionization can act as efficient proton donors and neutral CH3OH and HCO According to the theoretical calculations, the C-H bond cleavage in the radical cation should be more favorable than the O-H bo are observed and distinguished in the experiments with CD3OH and CH3OD. Our detailed mechanism of formation of the CH3O dot radicals contributes to understanding of astrochemistry in the protostellar medium.

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PubMed ID: 31322876

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Gamez, Francisco	P-7807-2018	0000-0001-6937-9950

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Record 66 of 235

Title: Surface Characterization of Colloidal Silica Nanoparticles by Second Harmonic Scattering: Quantifying the Surface Potent

Author(s): Marchioro, A (Marchioro, Arianna); Bischoff, M (Bischoff, Marie); Lutgebaucks, C (Luetgebaucks, Cornelis); Biriukov, D (Predota, Milan); Roke, S (Roke, Sylvie)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 123 **Issue:** 33 **Pages:** 20393-20404 **DOI:** 10.1021/acs.jpcc.9b05482 **Pub**

Abstract: The microscopic description of the interface of colloidal particles in solution is essential to understand and predict th well as their chemical and electrochemical reactivity. However, this description often relies on the use of simplified electrostatic structure of the interface, which give only theoretical estimates of surface potential values and do not provide properties relate structure, such as the orientation of interfacial water molecules. Here we apply polarimetric angle-resolved second harmonic s diameter SiO2 colloidal suspensions to experimentally determine both surface potential and interfacial water orientation as a f concentration. The surface potential values and interfacial water orientation change significantly over the studied pH and salt c zeta-potential (zeta) values remain constant. By comparing the surface and zeta-potentials, we find a layer of hydrated condens case, and for NaCl concentrations >= 1 mM. For milder pH ranges (pH < 11), as well as for salt concentrations <1 mM, no charge c observed. These findings are used to compute the surface charge densities using the Gouy-Chapman and Gouy-Chapman-Sterr using the AR-SHS data, we are able to determine the preferred water orientation in the layer directly in contact with the silica in simulations confirm the experimental trends and allow deciphering of the contributions of water layers to the total response.

Accession Number: WOS:000482545700036
Author Identifiers:

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

ISSN: 1932-7447
eISSN: 1932-7455

Record 67 of 235
Title: Ho2O@C-84: Crystallographic Evidence Showing Linear Metallic Oxide Cluster Encapsulated in IPR Fullerene Cage of D-2d
Author(s): Cong, HL (Cong, Hailin); Liu, A (Liu, Along); Hao, YJ (Hao, Yajuan); Feng, L (Feng, Lai); Slanina, Z (Slanina, Zdenek); Uh
Source: INORGANIC CHEMISTRY **Volume:** 58 **Issue:** 16 **Pages:** 10905-10911 **DOI:** 10.1021/acs.inorgchem.9b01318 **Published:** A
Abstract: Fullerene C-84 is the third-most-abundant species after C-60 and C-70. In the past decade, a variety of C-84-based clus studied experimentally, which otherwise do not include oxide clusterfullerenes (OCFs). In this work, we report a comprehensive including its mass, spectroscopic, crystallographic, electrochemical (EC), and density functional theory (DFT) studies. Importan reveal an IPR cage of D-2d(51591)-C-84 with a linear endohedral Ho-O-Ho cluster, indicating that the compression effect of the C compared to that of a smaller cage. The experimentally observed structure is confirmed by DFT computations, which also verify studies suggest that Ho2O@C-84 has reduced EC and HOMO-LUMO gaps compared to those of empty species, again demonstra encapsulation.
Accession Number: WOS:000482173300054
PubMed ID: 31356062
Author Identifiers:

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

ISSN: 0020-1669
eISSN: 1520-510X

Record 68 of 235
Title: Understanding structure and dynamics of organic liquid mixtures by molecular simulations
Author(s): Vokacova, ZS (Vokacova, Zuzana Sochorova); Pluharova, E (Pluharova, Eva)
Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 288 **Article Number:** UNSP 110778 **DOI:** 10.1016/j.molliq.2019.04.055 **Pu**
Abstract: The structure and dynamics of acetonitrile and its mixtures with toluene and water in the whole composition range ar dynamics simulations with several combinations of empirical non polarizable force fields. The acetonitrile and toluene binary s studied for the first time. One existing force field combination leads to unphysical phase separation in the mixture of acetonitril molar volumes, dielectric constants, viscosities and self-diffusion coefficients obtained by more suitable force fields are system experimental data. For static properties, it is possible to get nearly quantitative agreement for both kinds of mixtures. The evalu constant illustrates the importance of including the purely electronic component of polarization. The right trends for dynamica arrangement of the closest acetonitrile molecules is antiparallel in the neat liquid, those with slightly larger separation of molec respect to each other in various ways without strong preference for any of them. The addition of toluene causes structuring of a preference of antiparallel arrangement Water has a smaller effect on the acetonitrile radial distribution functions, but it affects t arrangements. (C) 2019 Elsevier B.V. All rights reserved.
Accession Number: WOS:000480664700072
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pluharova, Eva	B-1092-2012	

ISSN: 0167-7322
eISSN: 1873-3166

Record 69 of 235
Title: Opening up ROADMs: Let Us Build a Disaggregated Open Optical Line System
Author(s): Kundrat, J (Kundrat, Jan); Havlis, O (Havlis, Ondrej); Jedlinsky, J (Jedlinsky, Jaroslav); Vojtech, J (Vojtech, Josef)
Source: JOURNAL OF LIGHTWAVE TECHNOLOGY **Volume:** 37 **Issue:** 16 **Pages:** 4041-4051 **DOI:** 10.1109/JLT.2019.2906620 **Publi**

Abstract: At the lowest layer of today's communication networks is an optical line system (OLS), a physical network of equipme frequency analog light signals over thousands of kilometers. Traditionally, an OLS was delivered as a turn-key solution by a sing reconfigurable optical add/drop multiplexers (ROADMs) are active devices responsible for routing spectral chunks between inpu are arguably the most complex physical component of an OLS. In this paper, we describe an open design of a Czech Light ROAD hardware, electronics, software, and the northbound communication interface. The performance of the ROADMs is evaluated ir

Accession Number: WOS:000478943700022

Conference Title: OSA Photonic Networks and Devices (NETWORKS) Meeting

Conference Date: JUL 02-05, 2018

Conference Location: ETH Zurich, Zurich, SWITZERLAND

Conference Sponsors: OSA

Conference Host: ETH Zurich

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kundrat, Jan	Q-2021-2017	0000-0003-2957-9098

ISSN: 0733-8724

eISSN: 1558-2213

Record 70 of 235

Title: Quantum Yield Bias in Materials With Lower Absorptance

Author(s): van Dam, B (van Dam, Bart); Bruhn, B (Bruhn, Benjamin); Kondapaneni, I (Kondapaneni, Ivo); Dohnal, G (Dohnal, Gej Alexander); Krivanek, J (Krivanek, Jaroslav); Valenta, J (Valenta, Jan); Mudde, YD (Mudde, Yvo D.); Schall, P (Schall, Peter); Dohn Katerina)

Source: PHYSICAL REVIEW APPLIED **Volume:** 12 **Issue:** 2 **Article Number:** 024022 **DOI:** 10.1103/PhysRevApplied.12.024022 **Pu**

Abstract: Photoluminescence (PL) quantum yield (QY), which is defined as the ratio of emitted to absorbed photons, is the cent light-emitting materials. It is an important parameter to assess the light efficiency of new materials, as well as identify novel ph While QY measurements are performed as standard in research and industry, accurate measurements are challenging. Here, we inaccuracies, PL QY measurements exhibit a surprising systematic bias. QY values are underestimated by a factor of two or more absorption, which can even lead to misinterpretation of results. We combine PL QY measurements of diluted Rhodamine 6G an quantum dot solutions, via the standard integrating sphere method, with analytical modeling and ray-tracing simulations and f setup and luminescence mechanism, all measurements suffer from the same systematic underestimation of the QY. Through st measured emitted and absorbed photon numbers, we uncover the origin of this underestimation in the asymmetry of the ratio absorption, together with setup-specific features, such as signal offsets and nonlinearities. We suggest a robust calibration proc for precise evaluation of the QY in materials used for bioimaging, biosensing, and optoelectronic or photovoltaic devices.

Accession Number: WOS:000480400000003

Author Identifiers:

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Kondapaneni, Ivo	Q-1875-2017	0000-0003-2600-4416

ISSN: 2331-7019

Record 71 of 235

Title: Pore size effect on the separation of polymers by interaction chromatography. A Monte Carlo study

Author(s): Wang, X (Wang, Xiu); Prochazka, K (Prochazka, Karel); Limpouchova, Z (Limpouchova, Zuzana)

Source: ANALYTICA CHIMICA ACTA **Volume:** 1064 **Pages:** 126-137 **DOI:** 10.1016/j.aca.2019.03.017 **Published:** AUG 8 2019

Abstract: When the polymers are studied by interaction chromatography (IC) in porous media, the IC separation mechanism co exclusion chromatography (SEC) mechanism and under specific conditions close to the critical adsorption point (CAP), the elut polymer samples nonmonotonically depend on pore sizes. We performed Monte Carlo (MC) simulations to elucidate this intrigu behavior of self-avoiding and intersecting chains in twodimensionally (2D)-confining square pores and in 1D-confining slits in g confirmed that the dimensionality of the confinement, more specifically, pore geometry, controls the chromatographic behavic dependence of chromatographic characteristics on pore sizes occurs only in separations of self-avoiding chains on stationary p confining pores with strongly interacting walls. In agreement with experimental observations, the partition coefficient, K, increa narrow pores, peaks and then decreases in wider pores. The combination of thermodynamic and conformational analyses clea

interplay between enthalpy and entropy in 2D-confined media explains the nonmonotonic pore size dependence observed in tl specifies the region of conditions which endanger unambiguous interpretation of elution curves. Because the interplay of steric place not only in chromatography, but also in other separation techniques (e.g., gel electrophoresis, nanofluidic techniques), th relevant for all separations of large molecules in porous media. (C) 2019 Elsevier B.V. All rights reserved.

Accession Number: WOS:000464123500013

PubMed ID: 30982511

Author Identifiers:

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

ISSN: 0003-2670

eISSN: 1873-4324

Record 72 of 235

Title: Mossbauerite as Iron-Only Layered Oxyhydroxide Catalyst for WO3 Photoanodes

Author(s): Ertl, M (Ertl, Michael); Ma, ZL (Ma, Zili); Thersleff, T (Thersleff, Thomas); Lyu, PB (Lyu, Pengbo); Huettner, S (Huettner, (Nachtigall, Petr); Breu, J (Breu, Josef); Slabon, A (Slabon, Adam)

Source: INORGANIC CHEMISTRY **Volume:** 58 **Issue:** 15 **Pages:** 9655-9662 **DOI:** 10.1021/acs.inorgchem.9b00327 **Published:** AU

Abstract: Mossbauerite, a trivalent iron-only layered oxyhydroxide, has been recently identified as an electrocatalyst for water c material as potential cocatalyst for photoelectrochemical water oxidation on semiconductor photoanodes. The band edge posi determined for the first time with a combination of Mott-Schottky analysis and UV-vis diffuse reflectance spectroscopy. The pos Schottky slope and the flatband potential of 0.34 V vs reversible hydrogen electrode (RHE) identifies the material as an n-type s mossbauerite does not produce noticeable photocurrent during water oxidation. Type-II heterojunction formation by facile dro yielded photoanodes with amended charge carrier separation and photocurrents up to 1.22 mA cm(-2) at 1.23 V vs RHE. Mossba the charge carrier separation at lower potential and improving the photocurrent during photoelectrochemical water oxidation. the mossbauerite-functionalized WO3 photoanode thus originates from improved charge carrier separation and augmented ho results highlight the potential of mossbauerite as a second-phase catalyst for semiconductor electrodes.

Accession Number: WOS:000480371400020

PubMed ID: 31310522

Author Identifiers:

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Breu, Josef	G-7472-2019	0000-0002-2547-3950
Slabon, Adam	I-7780-2016	0000-0002-4452-1831

ISSN: 0020-1669

eISSN: 1520-510X

Record 73 of 235

Title: Bending of DNA duplexes with mutation motifs

Author(s): Ruzicka, M (Ruzicka, Michal); Soucek, R (Soucek, Remysl); Kulhanek, P (Kulhanek, Petr); Radova, L (Radova, Lenka); F Lenka); Reblova, K (Reblova, Kamila)

Source: DNA RESEARCH **Volume:** 26 **Issue:** 4 **Pages:** 341-352 **DOI:** 10.1093/dnares/dsz013 **Published:** AUG 2019

Abstract: Mutations can be induced by environmental factors but also arise spontaneously during DNA replication or due to dea cytosines at CpG dinucleotides. Sites where mutations occur with higher frequency than would be expected by chance are term contain mutations rarely are termed coldspots. Mutations are permanently scanned and repaired by repair systems. Among the targets base pair mismatches, which are discriminated from canonical base pairs by probing altered elasticity of DNA. Using bia simulations, we investigated the elasticity of coldspots and hotspots motifs detected in human genes associated with inherited with Czech population hotspots and de novo mutations. Main attention was paid to mutations leading to G/T and A+/C pairs. W without CpG/CpHpG sequences are less flexible than coldspots, which indicates that flexible sequences are more effectively rep with CpG/CpHpG sequences exhibited increased flexibility as coldspots. Their mutability is more likely related to spontaneous c cytosines leading to C > T mutations, which are primarily targeted by base excision repair. We corroborated conclusions based c measuring melting curves of hotspots and coldspots containing G/T mismatch.

Accession Number: WOS:000493011000005

PubMed ID: 31230075
ISSN: 1340-2838
eISSN: 1756-1663

Record 74 of 235

Title: Distributed sources as a cause of abrupt amplitude decrease in cubic distortion-product otoacoustic emissions at high sti
Author(s): Vencovsky, V (Vencovsky, Vaclav); Vetesnik, A (Vetesnik, Ales); Dalhoff, E (Dalhoff, Ernst); Gummer, AW (Gummer, Anth
Source: JOURNAL OF THE ACOUSTICAL SOCIETY OF AMERICA **Volume:** 146 **Issue:** 2 **Pages:** EL92-EL98 **DOI:** 10.1121/1.5119942
Abstract: The amplitudes of distortion-product otoacoustic emissions (DPOAEs) may abruptly decrease even though the stimul These notches observed in the DPOAE input/output functions or distortion-product grams have been hypothesized to be due to between wavelets generated by distributed sources of the nonlinear-distortion component of DPOAEs. In this paper, simulation model and its analytical solution support the hypothesis that destructive interference between individual wavelets may lead to explain the cause for onset and offset amplitude overshoots in the DPOAE signal measured for intensity pairs in the notches.
Accession Number: WOS:000483887400002
PubMed ID: 31472590
ISSN: 0001-4966
eISSN: 1520-8524

Record 75 of 235

Title: FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabo
Author(s): Sicho, M (Sicho, Martin); Stork, C (Stork, Conrad); Mazzolari, A (Mazzolari, Angelica); Kops, CD (Kops, Christina de Bru Alessandro); Testa, B (Testa, Bernard); Vistoli, G (Vistoli, Giulio); Svozil, D (Svozil, Daniel); Kirchmair, J (Kirchmair, Johannes)
Source: JOURNAL OF CHEMICAL INFORMATION AND MODELING **Volume:** 59 **Issue:** 8 **Pages:** 3400-3412 **DOI:** 10.1021/acs.jcim.9 2019
Abstract: In this work we present the third generation of FAst MEtabolizer (FAME 3), a collection of extra trees classifiers for the p metabolism (SoMs) in small molecules such as drugs, druglike compounds, natural products, agrochemicals, and cosmetics. FA MetaQSAR database (Pedretti et al. J. Med. Chem. 2018, 61, 1019), a recently published data resource on xenobiotic metabolism substrates annotated with more than 6300 experimentally confirmed SoMs related to redox reactions, hydrolysis and other non conjugation reactions. In tests with holdout data, FAME 3 models reached competitive performance, with Matthews correlation from 0.50 for a global model covering phase 1 and phase 2 metabolism, to 0.75 for a focused model for phase 2 metabolism. A n P450 metabolism yielded an MCC of 0.57. Results from case studies with several synthetic compounds, natural products, and na demonstrate the agreement between model predictions and literature data even for molecules with structural patterns clearly the training data. The applicability domains of the individual models were estimated by a new, atom-based distance measure (I nearest-neighbor search in the space of atom environments. FAME 3 is available via a public web service at https://nerdd.zbh.u contained Java software package, free for academic and noncommercial research.
Accession Number: WOS:000483436400006
PubMed ID: 31361490
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ISSN: 1549-9596
eISSN: 1549-960X

Record 76 of 235

Title: Polymeric hollow fibers: Uniform temperature of Li-ion cells in battery modules
Author(s): Bohacek, J (Bohacek, Jan); Raudensky, M (Raudensky, Miroslav); Karimi-Sibaki, E (Karimi-Sibaki, Ebrahim)
Source: APPLIED THERMAL ENGINEERING **Volume:** 159 **Article Number:** UNSP 113940 **DOI:** 10.1016/j.applthermaleng.2019.11
Abstract: In the present work, a new heat exchanger is introduced for conventional liquid cooling of cylindrical type lithium-ion battery packs/modules of electric vehicles. The coolant channels are made of polymeric hollow fibers (empty set 1 mm) embed polydicyclopentadiene housing. Unlike commercially available metallic counterparts, the proposed design is lightweight, elect

made of low cost materials. The prototype is stacked with 18650-type lithium-ion cells which are cycled with 1 C in the range of and 100%. Water/coolant circulates in the hollow fibers in the range of 0.1-0.71/min corresponding to the flow rate supplied to a kilowatt hour of electrical energy. For the coolant temperature of 23 degrees C at the inlet, maximum temperature of the hottes degrees C in the given range of flow rates. Furthermore, temperature spread among cells is in the range between 14.6 and 4.6 d mathematical optimization coupled with computational fluid dynamics simulations, we found that having a homogeneous tem all the Li-ion cells is achievable. For that purpose, a non-uniform thickness of thermal insulation is suggested. The temperature a given flow rate of the coolant and even when temporal variations in the heat generation rate occur.

Accession Number: WOS:000475999100110

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Bohacek, Jan	C-2078-2018	0000-0003-3319-4254

ISSN: 1359-4311

Record 77 of 235

Title: Maximum N content in a-CNx by ab-initio simulations

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

Source: ACTA MATERIALIA **Volume:** 174 **Pages:** 189-194 **DOI:** 10.1016/j.actamat.2019.05.048 **Published:** AUG 1 2019

Abstract: Structures of amorphous CN, materials are predicted by extensive ab-initio molecular-dynamics simulations (more th range of compositions and densities. The main attention is paid to the formation of N-2 molecules, with the aim to predict and content in stable CNx networks. The results show that the maximum N content is of approximate to 42 at.%. From the kinetics p contents lead to steeply increasing rate of N-2 formation during materials formation. From the thermodynamics point of view, h may be temporarily stabilized by N-2 molecules sitting in voids around the network, but a subsequent N-2 diffusion into the atn unstable. The results are important for the design of CNx (and other nitride) materials and pathways for their preparation for va applications. (C) 2019 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Accession Number: WOS:000474501300018

Author Identifiers:

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

ISSN: 1359-6454

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Record 78 of 235

Title: Synthesis and structural characterisation of 1'-(diphenylphosphino) ferrocene-1-phosphonic acid, its ammonium salts an

Author(s): Horky, F (Horky, Filip); Cisarova, I (Cisarova, Ivana); Schulz, J (Schulz, Jiri); Stepnicka, P (Stepnicka, Petr)

Source: JOURNAL OF ORGANOMETALLIC CHEMISTRY **Volume:** 891 **Pages:** 44-53 **DOI:** 10.1016/j.jorganchem.2019.04.012 **Publi**

Abstract: A new polar phosphinoferrocene ligand, viz. 1'-(diphenylphosphino)ferrocene-1-phosphonic acid (H2L), was prepared corresponding phosphonate ethyl ester. However, the compound is relatively unstable, gradually decomposing upon prolonged phosphine oxide H2LO. When the phosphine moiety was protected (e.g., in phosphine oxide H2LO and adduct H2L center dot B observed. An alternative approach to prepare more stable H2L surrogates by converting the phosphonic acid into ammonium s [(OHCH2CH2)(2)NH2](HL) (dabco = 1,4-diazabicyclo[2.2.2]octane) resulted in no significant stabilisation. H2L reacted with [PdC diene), producing the bis(phosphine) complex, trans-[PdCl2(H2L-kappa P)(2)]. When mixed with Pd(II)-acetylacetonate (acac) c metallated auxiliary ligands, [(L-CY)Pd(acac)] (L-CY = 2-[(dimethylamino-kappa N)methyl]phenyl-kappa C-1 and 2-[(methylthio- kappa C-1), H2L gave rise to bis-chelate complexes of the [(L-CY)Pd(HL-kappa O-2,P)] type. H2L, the ammonium salts featuring t complexes were structurally characterised by single-crystal X-ray diffraction analysis. Variations in phosphonate P-O bond lengt structures were rationalised by DFT computations. (C) 2019 Elsevier B.V. All rights reserved.

Accession Number: WOS:000466789300007

Author Identifiers:

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Stepnicka, Petr	E-3465-2010	0000-0002-5966-0578

ISSN: 0022-328X

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Record 79 of 235

Title: Structures of Peptidic H-wires at Mercury Surface: Molecular Dynamics Study

Author(s): Kroutil, O (Kroutil, Ondrej); Kabelac, M (Kabelac, Martin); Dorcak, V (Dorcak, Vlastimil); Vacek, J (Vacek, Jan)

Source: ELECTROANALYSIS **Volume:** 31 **Issue:** 10 **Special Issue:** SI **Pages:** 2032-2040 **DOI:** 10.1002/elan.201900314 **Early Acce** OCT 2019

Abstract: Biopolymer immobilization strategies, self-assembly systems and adsorption phenomenon in general are crucial for t that work on the basis of the surface-detection principle, including electrochemistry. A mechanistic view into the interaction of surfaces is also important for studying fundamental and dynamic processes such as electron/proton transport. In this sense, th approaches for investigating the interfacial behavior of immobilized biomolecular architectures is a permanent focus. Here we (MD) approach to simulate the structural changes and metallic surface interactions of a model 21-mer peptide of His (H) and Ala proton wire (H-wire). This H-wire was previously proposed for the electrochemical study of proton transfer at mercury electrode The rigid solid mercury mono-atomic layer (alpha-mercury lattice model) was used systematically in all our simulations. The ca a simulation box with 1, 16 and 32 H-wire strands attached covalently to the mercury layer via the thiol group of a cysteinamide H-wire C-terminus. The internal alpha-helical configuration of H-wires was maintained by the presence of 2,2,2-trifluoroethanol surface density of H-wires and the protonation state of His residues play a decisive role in the structural stability and orientation whereas the applied voltage only has a mild effect on it, especially in case of 16 and 32 H-wire strand configurations. The MD sin could be used for the further investigation of other peptides at metallic surfaces and for electrochemical analyses of structural c peptides that depend on their protonation states and other external factors.

Accession Number: WOS:000479714500001

ISSN: 1040-0397

eISSN: 1521-4109

Record 80 of 235

Title: Directly Sequenced Genomes of Contemporary Strains of Syphilis Reveal Recombination-Driven Diversity in Genes Encod Exposed Antigens

Author(s): Grillova, L (Grillova, Linda); Oppelt, J (Oppelt, Jan); Mikalova, L (Mikalova, Lenka); Novakova, M (Novakova, Marketa); Niesnerova, A (Niesnerova, Anezka); Noda, AA (Noda, Angel A.); Mechaly, AE (Mechaly, Ariel E.); Pospisilova, P (Pospisilova, Petra Darina); Grange, PA (Grange, Philippe A.); Dupin, N (Dupin, Nicolas); Strnadel, R (Strnadel, Radim); Chen, M (Chen, Marcus); Denl (Arora, Natasha); Picardeau, M (Picardeau, Mathieu); Weston, C (Weston, Christopher); Forsyth, RA (Forsyth, R. Allyn); Smajs, D (S

Source: FRONTIERS IN MICROBIOLOGY **Volume:** 10 **Article Number:** 1691 **DOI:** 10.3389/fmicb.2019.01691 **Published:** JUL 31 2

Abstract: Syphilis, caused by Treponema pallidum subsp. pallidum (TPA), remains an important public health problem with an prevalence. Despite recent advances in in vitro cultivation, genetic variability of this pathogen during infection is poorly underst contemporary and geographically diverse complete treponemal genome sequences isolated directly from patients using a metl to sequencing. This approach reveals that approximately 50% of the genetic diversity found in TPA is driven by inter- and/or intr events, particularly in strains belonging to one of the defined genetic groups of syphilis treponemes: Nichols-like strains. Recom encode putative outer-membrane proteins and the recombination variability was almost exclusively found in regions predicted interface. Genetic recombination has been considered to be a rare event in treponemes, yet our study unexpectedly showed tha level and may have important impacts in the biology of this pathogen, especially as these events occur primarily in the outer m reveals the existence of strains with different repertoires of surface-exposed antigens circulating in the current human populati into account during syphilis vaccine development.

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PubMed ID: 31417509

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ISSN: 1664-302X

Record 81 of 235

Title: Electron transport in high-entropy alloys: AlxCrFeCoNi as a case study

Author(s): Kudrnovsky, J (Kudrnovsky, J.); Drchal, V (Drchal, V); Maca, F (Maca, F.); Turek, I (Turek, I); Khmelevskyi, S (Khmelevsk

Source: PHYSICAL REVIEW B **Volume:** 100 **Issue:** 1 **Article Number:** 014441 **DOI:** 10.1103/PhysRevB.100.014441 **Published:** JU

Abstract: The high-entropy alloys AlxCrFeCoNi exist over a broad range of Al concentrations (0 < x < 2). With increasing Al conter from the fcc to bcc phase. We investigate the effect of such structural changes on transport properties including the residual res Hall resistivity. We have performed a detailed comparison of the first-principles simulations with available experimental data. W residual resistivities for all studied alloy compositions are in a fair agreement with available experimental data as concerns both concentration trends. We emphasize that a good agreement with experiment was obtained also for the anomalous Hall resistivi by estimation of the anisotropic magnetoresistance, spin-disorder resistivity, and Gilbert damping. The obtained results prove t mechanism is due to the intrinsic chemical disorder whereas the effect of spin polarization on the residual resistivity is appreci

Accession Number: WOS:000478041100002

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Khmelevskyi, Sergii	T-1192-2017	0000-0001-5630-7835

ISSN: 2469-9950

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Record 82 of 235

Title: Molecular and biological properties of two putative new cytorhabdoviruses infecting Trifolium pratense

Author(s): Franova, J (Franova, J.); Sarkisova, T (Sarkisova, T.); Jakesova, H (Jakesova, H.); Koloniuk, I (Koloniuk, I)

Source: PLANT PATHOLOGY **DOI:** 10.1111/ppa.13065 **Early Access Date:** JUL 2019

Abstract: Three pairs of generic primers designed for specific reverse transcription polymerase chain reaction amplification of p genomes were successfully tested with a number of red clover samples. Two infected plants showing irregular vein clearing, tiss growth symptoms were selected for further studies. Subsequently, two novel plant rhabdoviruses, tentatively named Trifolium Trifolium pratense virus B (TpVB), were detected in red clover plants. Sequence analyses of nucleotide sequences of their genor throughput sequencing confirmed their affinity to members of the genus Cytorhabdovirus. While TpVA was transmitted by mec Nicotiana occidentalis 37B and subtransferred to Physalis floridana plants, crude sap transmission of TpVB to a range of herbac bacilliform shape of virions, which has a cytoplasm-limited distribution, their sizes, and the phylogenetic relationships, suppor TpVB to two distinct species of the genus Cytorhabdovirus.

Accession Number: WOS:000479420000001

Author Identifiers:

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Koloniuk, Igor	X-5540-2019	0000-0002-5893-6683
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ISSN: 0032-0862

eISSN: 1365-3059

Record 83 of 235

Title: Mass spectrometric investigation of amorphous Ga-Sb-Se thin films

Author(s): Mawale, R (Mawale, Ravi); Halenkovic, T (Halenkovic, Tomas); Bouska, M (Bouska, Marek); Gutwirth, J (Gutwirth, Jan Virginie); Bora, PL (Bora, Pankaj Lochan); Pecinka, L (Pecinka, Lukas); Prokes, L (Prokes, Lubomir); Havel, J (Havel, Josef); Neme

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 10213 **DOI:** 10.1038/s41598-019-46767-8 **Published:** JUL 15 2019

Abstract: Amorphous chalcogenide thin films are widely studied due to their enhanced properties and extensive applications. H amorphous Ga-Sb-Se chalcogenide thin films prepared by magnetron co-sputtering, via laser ablation quadrupole ion trap time Furthermore, the stoichiometry of the generated clusters was determined which gives information about individual species pre originating from the interaction of amorphous chalcogenides with high energy laser pulses. Seven different compositions of thi at. %, Sb content 5.2-31.2 at. %, Se content 61.2-63.3 at. %) were studied and in each case about -50 different clusters were ider clusters in negative ion mode. Assuming that polymers can influence the laser desorption (laser ablation) process, we have use reduce the destruction of the amorphous network structure and/or promote the laser ablation synthesis of heavier species fron case, many new and higher mass clusters were identified. The maximum number of (40) new clusters was detected for the Ga-S highest amount of antimony (31.2 at. %). This approach opens new possibilities for laser desorption ionization/laser ablation st Finally, for selected binary and ternary clusters, their structure was calculated by using density functional theory optimization p

Accession Number: WOS:000475467800056

PubMed ID: 31308483
ISSN: 2045-2322

Record 84 of 235

Title: Interface dipoles of Ir(ppy)(3) on Cu(111)

Author(s): Queck, F (Queck, Fabian); Albrecht, F (Albrecht, Florian); Mutombo, P (Mutombo, Pingo); Krejci, O (Krejci, Ondrej); Je McLean, A (McLean, Alastair); Repp, J (Repp, Jascha)

Source: NANOSCALE **Volume:** 11 **Issue:** 26 **Pages:** 12695-12703 **DOI:** 10.1039/c9nr00934e **Published:** JUL 14 2019

Abstract: The interplay of adsorption geometry and interface dipoles of the transition-metal complex Ir(ppy)(3) on Cu(111) was temperature scanning probe microscopy and density-functional-theory calculations. We find that the orientation of the molecu with respect to the surface has a strong influence on the total energy of the different configurations, where the most stable one moment pointing out of the surface plane along the surface normal. Adsorption-induced redistribution of charges results in an that also points out of the surface plane for all configurations. Submolecularly resolved maps of the resulting local contact pote any in-plane dipole moment is very effectively screened.

Accession Number: WOS:000474160000028
PubMed ID: 31240287
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Queck, Fabian		0000-0001-6596-7229

ISSN: 2040-3364
eISSN: 2040-3372

Record 85 of 235

Title: Identifying the molecular adsorption site of a single molecule junction through combined Raman and conductance studie

Author(s): Kaneko, S (Kaneko, Satoshi); Montes, E (Montes, Enrique); Suzuki, S (Suzuki, Sho); Fujii, S (Fujii, Shintaro); Nishino, T Tsukagoshi, K (Tsukagoshi, Kazuhito); Ikeda, K (Ikeda, Katsuyoshi); Kano, H (Kano, Hideaki); Nakamura, H (Nakamura, Hisao); Va Kiguchi, M (Kiguchi, Manabu)

Source: CHEMICAL SCIENCE **Volume:** 10 **Issue:** 25 **Pages:** 6261-6269 **DOI:** 10.1039/c9sc00701f **Published:** JUL 7 2019

Abstract: Single-molecule junctions are ideal test beds for investigating the fundamentals of charge transport at the nanoscale. strongly dependent on the metal-molecule interface geometry, which, however, is very poorly characterized due to numerous e report on a new methodology for characterizing the adsorption site of single-molecule junctions through the combination of su scattering (SERS), current-voltage (I-V) curve measurements, and density functional theory simulations. This new methodology different adsorption sites for benzenedithiol and aminobenzenethiol junctions, which cannot be identified by solo measureme curves. Using this methodology, we determine the interface geometry of these two prototypical molecules at the junction and i modulating the applied voltage, we can change and monitor the distribution of adsorption sites at the junction.

Accession Number: WOS:000473055300021
PubMed ID: 31367301
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Author	Web of Science ResearcherID	ORCID Number
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Fujii, Shintaro	B-4779-2011	0000-0003-2869-7674

ISSN: 2041-6520
eISSN: 2041-6539

Record 86 of 235

Title: Sequence Versus Composition: What Prescribes IDP Biophysical Properties?

Author(s): Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri); Hlouchova, K (Hlouchova, Klara)

Source: ENTROPY **Volume:** 21 **Issue:** 7 **Article Number:** 654 **DOI:** 10.3390/e21070654 **Published:** JUL 2019

Abstract: Intrinsically disordered proteins (IDPs) represent a distinct class of proteins and are distinguished from globular prote plasticity, high evolvability and a broad functional repertoire. Some of their properties are reminiscent of early proteins, but the functional properties and compositional bias suggest that IDPs appeared at later evolutionary stages. The spectrum of IDP prop are still not well defined. This study compares rudimentary physicochemical properties of IDPs and globular proteins using bioi level of their native sequences and random sequence permutations, addressing the contributions of composition versus seque properties. IDPs have, on average, lower predicted secondary structure contents and aggregation propensities and biased amir However, our study shows that IDPs exhibit a broad range of these properties. Induced fold IDPs exhibit very similar compositio structure/aggregation propensities to globular proteins, and can be distinguished from unfoldable IDPs based on analysis of th While amino acid composition seems to be a major determinant of aggregation and secondary structure propensities, sequenc result in dramatic changes to these properties, but for both IDPs and globular proteins seems to fine-tune the tradeoff between

Accession Number: WOS:000478585200086

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Hlouchova, Klara	G-9531-2017	0000-0002-5651-4874

eISSN: 1099-4300

Record 87 of 235

Title: Structural basis for the multitasking nature of the potato virus Y coat protein

Author(s): Kezar, A (Kezar, Andreja); Kavcic, L (Kavcic, Luka); Polak, M (Polak, Martin); Novacek, J (Novacek, Jiri); Gutierrez-Aguir Znidaric, MT (Znidaric, Magda Tusek); Co, A (Co, Anna); Stare, K (Stare, Katja); Gruden, K (Gruden, Kristina); Ravnikar, M (Ravnika (Pahovnik, David); Zagar, E (Zagar, Ema); Merzel, F (Merzel, Franci); Anderluh, G (Anderluh, Gregor); Podobnik, M (Podobnik, Mar

Source: SCIENCE ADVANCES **Volume:** 5 **Issue:** 7 **Article Number:** eaaw3808 **DOI:** 10.1126/sciadv.aaw3808 **Published:** JUL 201

Abstract: Potato virus Y (PVY) is among the most economically important plant pathogens. Using cryoelectron microscopy, we d structure of PVY's flexuous virions, revealing a previously unknown lumenal interplay between extended carboxyl-terminal regi and viral RNA. RNA-coat protein interactions are crucial for the helical configuration and stability of the virion, as revealed by th structure of RNA-free virus-like particles. The structures offer the first evidence for plasticity of the coat protein's amino- and ca Together with mutational analysis and in planta experiments, we show their crucial role in PVY infectivity and explain the ability perform multiple biological tasks. Moreover, the high modularity of PVY virus-like particles suggests their potential as a new mo nanobiotechnological applications.

Accession Number: WOS:000478770400067

PubMed ID: 31328164

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ISSN: 2375-2548

Record 88 of 235

Title: Comparability of long-term temporal trends of POPs from co-located active and passive air monitoring networks in Europ

Author(s): Kalina, J (Kalina, Jiri); White, KB (White, Kevin B.); Scheringer, M (Scheringer, Martin); Pribylova, P (Pribylova, Petra); Audy, O (Audy, Ondrej); Klanova, J (Klanova, Jana)

Source: ENVIRONMENTAL SCIENCE-PROCESSES & IMPACTS **Volume:** 21 **Issue:** 7 **Pages:** 1132-1142 **DOI:** 10.1039/c9em00136k

Abstract: The comparability of data from active (ACT) and passive sampling (PAS) of persistent organic pollutants (POPs) in air i related to the derivation of sampling rates and concentrations, as well as differences in the duration, volume and frequency of s ACT have been used extensively in short-term PAS calibration studies, no attempts have been made to evaluate the comparabili calculated from PAS to established ACT trends. This is crucial, as continuous long-term ACT is unfeasible in most regions of the v challenges, we calculated and compared trends for organochlorine pesticides (OCPs), polychlorinated biphenyls (PCBs) and po (PBDEs) at the six sites in Europe with at least 5 years of co-located ACT and PAS data (2012-2016): Birkenes, Kosetice, Pallas, Ra

Strong agreement of ACT and PAS trends was observed for most OCPs and PCBs. Apart from two PCBs at Storhofoi, all pairs of A the same direction. However, differences in the magnitude, significance and confidence intervals of their slopes were observed were primarily attributed to the short duration of the PAS time series. Despite some limitations, our results suggest that the con POP trends will continue to improve with additional years of data. This study confirms the suitability of PAS for the calculation o and highlights the importance of continuous sampling at established monitoring sites with consistent analytical methods.

Accession Number: WOS:000475800200004

PubMed ID: 31245802

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 2050-7887

eISSN: 2050-7895

Record 89 of 235

Title: Studies of laser-plasma interaction physics with low-density targets for direct-drive inertial confinement schemes

Author(s): Tikhonchuk, V (Tikhonchuk, V); Gu, YJ (Gu, Y. J.); Klimo, O (Klimo, O.); Limpouch, J (Limpouch, J.); Weber, S (Weber, S

Source: MATTER AND RADIATION AT EXTREMES **Volume:** 4 **Issue:** 4 **Article Number:** UNSP 045402 **DOI:** 10.1063/1.5090965 **Pu**

Abstract: Comprehensive understanding and possible control of parametric instabilities in the context of inertial confinement f challenging task. The details of the absorption processes and the detrimental effects of hot electrons on the implosion process experimental side as on the theoretical and simulation side. This paper describes a proposal for experimental studies on nonlin laser pulses with a high-temperature plasma under conditions corresponding to direct-drive ICF schemes. We propose to devel interaction studies based on foam targets. Parametric instabilities are sensitive to the bulk plasma temperature and the density are sufficiently flexible to allow control of these parameters. However, investigations conducted on small laser facilities cannot way to real fusion conditions. It is therefore necessary to perform experiments at a multi-kilojoule energy level on medium-scal SG-III. An example of two-plasmon decay instability excited in the interaction of two laser beams is considered. (C) 2019 Author

Accession Number: WOS:000475743800005

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Tikhonchuk, Vladimir	S-1160-2018	0000-0001-7532-5879

ISSN: 2468-2047

eISSN: 2468-080X

Record 90 of 235

Title: The Bronsted acidity of three- and two-dimensional zeolites

Author(s): Thang, HV (Ho Viet Thang); Vaculik, J (Vaculik, Jan); Prech, J (Prech, Jan); Kubu, M (Kubu, Martin); Cejka, J (Cejka, Jir Petr); Bulanek, R (Bulanek, Roman); Grajciar, L (Grajciar, Lukas)

Source: MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 282 **Pages:** 121-132 **DOI:** 10.1016/j.micromeso.2019.03.033 **P**

Abstract: The zeolite activity in processes driven by Bronsted acid sites is determined by the distribution of the protons in the ze interaction with the framework. This study aims to assess how much the transformation from three-dimensional (3D) bulk zeoli dimensional (2D) layered form changes the proton distribution and strength of the proton-framework interaction and thus how Bronsted acid strength. Zeolites with three distinct topologies, MWW, PCR, and MFI, which form also layered analogues with cor and silanol density were considered. To probe the Bronsted acidity of both 3D and 2D forms, an array of typical acidity descripto frequency, shift of O-H frequencies upon adsorption of CO probe molecule, C-O stretching frequencies and adsorption enthalpi complex) have been evaluated, employing both dispersion-corrected density functional theory and Fourier-transform infrared s descriptors, the Bronsted acidity of 2D form is, on average, the same or just slightly lower than that of the 3D form. Transformat affect the proton distribution and values of acidity descriptors for individual T sites, however, if all T sites are considered, the ag negligible. Hence, these results suggest that a larger effect of the 3D - > 2D transformation can be expected for frameworks with

Accession Number: WOS:000471206400016

Author Identifiers:

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Cejka, Jiri	B-1833-2013	0000-0003-1400-1031

ISSN: 1387-1811

eISSN: 1873-3093

Record 91 of 235

Title: Sample size for maximum-likelihood estimates of Gaussian model depending on dimensionality of pattern space

Author(s): Psutka, JV (Psutka, Josef V.); Psutka, J (Psutka, Josef)

Source: PATTERN RECOGNITION **Volume:** 91 **Pages:** 25-33 **DOI:** 10.1016/j.patcog.2019.01.046 **Published:** JUL 2019

Abstract: The significant properties of the maximum likelihood (ML) estimate are consistency, normality, and efficiency. While it properties are valid when the sample size approaches infinity, the behavior of an ML estimator when working with small sample However, in real tasks, we usually do not have sufficient data to completely fulfill the conditions of an optimal ML estimate. The amount of data is required to be able to estimate a Gaussian model that provides sufficiently accurate likelihood estimates. This respect to the number of dimensions of the pattern space. (C) 2019 Elsevier Ltd. All rights reserved.

Accession Number: WOS:000466250400003

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Psutka, Josef		0000-0003-4761-1645

ISSN: 0031-3203

eISSN: 1873-5142

Record 92 of 235

Title: Calculated relative populations for the Eu@C-82 isomers

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

Source: CHEMICAL PHYSICS LETTERS **Volume:** 726 **Pages:** 29-33 **DOI:** 10.1016/j.cplett.2019.04.011 **Published:** JUL 2019

Abstract: Relative populations of four IPR (isolated-pentagon-rule) isomers of Eu@C-82 are computed using the Gibbs energy b density functional theory calculations (M06-2X/6-31G*similar to SDD entropy term, M06-2X/6-31+G*similar to SDD or B2PLYPD/6 energetics). Only the species observed by now also show significant calculated populations. A role of solubility in different solve the arc electrodes could explain variability in the observed populations.

Accession Number: WOS:000466852600006

ISSN: 0009-2614

eISSN: 1873-4448

Record 93 of 235

Title: Varroa destructor parasitism has a greater effect on proteome changes than the deformed wing virus and activates TGF-b

Author(s): Erban, T (Erban, Tomas); Sopko, B (Sopko, Bruno); Kadlikova, K (Kadlikova, Klara); Talacko, P (Talacko, Pavel); Haran

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 9400 **DOI:** 10.1038/s41598-019-45764-1 **Published:** JUN 28 2019

Abstract: Honeybee workers undergo metamorphosis in capped cells for approximately 13 days before adult emergence. Durin mites prick the defenseless host many times. We sought to identify proteome differences between emerging Varroa-parasitized showing the presence or absence of clinical signs of deformed wing virus (DWV) in the capped cells. A label-free proteomic anal with an Orbitrap Fusion Tribrid mass spectrometer provided a quantitative comparison of 2316 protein hits. Redundancy analys combination of Varroa parasitism and DWV clinical signs caused proteome changes that occurred in the same direction as those approximately two-fold higher. Furthermore, proteome changes associated with DWV signs alone were positioned above Varroa indicate that Varroa activates TGF-beta-induced pathways to suppress wound healing and the immune response and that the c intensifies these effects. Furthermore, we indicate JAK/STAT hyperactivation, p53-BCL-6 feedback loop disruption, Wnt pathway crosstalk disruption, and NF-kappa B and JAK/STAT signaling conflict in the Varroa-honeybee-DWV interaction. These results illu Varroa than of DWV at the time of emergence. Markers for future research are provided.

Accession Number: WOS:000473130000021

PubMed ID: 31253851

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sopko, Bruno	N-7345-2018	0000-0002-5580-1871
Erban, Tomas	F-9615-2011	0000-0003-1730-779X

ISSN: 2045-2322

Record 94 of 235

Title: Separation of polymers differing in their chain architecture by interaction chromatography: Phase equilibria and conform in strongly adsorbing porous media

Author(s): Wang, X (Wang, Xiu); Limpouchova, Z (Limpouchova, Zuzana); Prochazka, K (Prochazka, Karel)

Source: POLYMER **Volume:** 175 **Pages:** 99-106 **DOI:** 10.1016/j.polymer.2019.05.006 **Published:** JUN 26 2019

Abstract: Understanding the competition between adsorption on confining interfaces and conformational behavior of polymer necessary condition for correct interpretation of chromatographic curves. Accordingly, we investigated the conformational beh polymers and the impact of the chain architecture on phase equilibria in porous media using Monte Carlo (MC) simulations. We chromatography (IC) under conditions close to the critical adsorption point (CAP). We evaluated the concentration-dependent and used them as an input for the solution of a time-discretized mass balance equation which predicts the shapes of the elutio the effects of chain architecture on the IC separation mechanism and shows that IC is a promising method for the separation of

Accession Number: WOS:000471252600013

Author Identifiers:

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

ISSN: 0032-3861

eISSN: 1873-2291

Record 95 of 235

Title: High-throughput analysis revealed mutations' diverging effects on SMN1 exon 7 splicing

Author(s): Soucek, P (Soucek, Premysl); Reblova, K (Reblova, Kamila); Kramarek, M (Kramarek, Michal); Radova, L (Radova, Len Tereza); Hujova, P (Hujova, Pavia); Kovacova, T (Kovacova, Tatiana); Lexa, M (Lexa, Matej); Grodecka, L (Grodecka, Lucie); Freibe

Source: RNA BIOLOGY **Volume:** 16 **Issue:** 10 **Pages:** 1364-1376 **DOI:** 10.1080/15476286.2019.1630796 **Early Access Date:** JUN 2

Abstract: Splicing-affecting mutations can disrupt gene function by altering the transcript assembly. To ascertain splicing dysre modified a minigene assay for the parallel high-throughput evaluation of different mutations by next-generation sequencing. In and six intronic positions of the SMN1 gene's exon 7 were mutated to all possible nucleotide variants, which amounted to 180 u mutants and 470 double mutants. The mutations resulted in a wide range of splicing aberrations. Exonic splicing-affecting muta substantial exon skipping, supposedly driven by predicted exonic splicing silencer or cryptic donor splice site (5 ' ss) and de nov use. On the other hand, a single disruption of exonic splicing enhancer was not sufficient to cause major exon skipping, suggest substituted during exon recognition. While disrupting the acceptor splice site led only to exon skipping, some 5 ' ss mutations p different cryptic 5 ' ss. Generally, single mutations supporting cryptic 5 ' ss use displayed better pre-mRNA/U1 snRNA duplex sta regulatory element strength across the original 5 ' ss. Analyzing double mutants supported the predominating splicing regulatc snRNA binding could contribute to the global balance of splicing isoforms. Based on these findings, we suggest that creating a r the mutated 5 ' ss can be one of the main factors driving cryptic 5 ' ss use.

Accession Number: WOS:000472379600001

PubMed ID: 31213135

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ISSN: 1547-6286

eISSN: 1555-8584

Record 96 of 235

Title: Oscillatory migration of accreting protoplanets driven by a 3D distortion of the gas flow

Author(s): Chrenko, O (Chrenko, Ondrej); Lambrechts, M (Lambrechts, Michiel)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 626 **Article Number:** A109 **DOI:** 10.1051/0004-6361/201935334 **Published:** JU
Abstract: Context. The dynamics of a low-mass protoplanet accreting solids is influenced by the heating torque, which was four migration in protoplanetary disks with constant opacities.
Aims. We investigate the differences in the heating torque between disks with constant and temperature-dependent opacities.
Methods. Interactions of a super-Earth-sized protoplanet with the gas disk are explored using 3D radiation hydrodynamic simul
Results. Accretion heating of the protoplanet creates a hot underdense region in the surrounding gas, leading to misalignment pressure gradients. As a result, the 3D gas flow is perturbed and some of the streamlines form a retrograde spiral rising above th constant-opacity disk, the perturbed flow reaches a steady state and the underdense gas responsible for the heating torque ren accordance with previous studies. If the opacity is non-uniform, however, the differences in the disk structure can lead to more and eventually to a flow instability. The underdense gas develops a one-sided asymmetry which circulates around the protopla The heating torque thus strongly oscillates in time and does not on average counteract inward migration.
Conclusions. The torque variations make the radial drift of the protoplanet oscillatory, consisting of short intervals of alternatin migration. We speculate that transitions between the positive and oscillatory heating torque may occur in specific disk regions convection, resulting in the convergent migration of multiple planetary embryos.
Accession Number: WOS:000472130500001
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Author	Web of Science ResearcherID	ORCID Number
Chrenko, Ondrej	W-4258-2019	0000-0001-7215-5026

ISSN: 1432-0746

Record 97 of 235

Title: Do star clusters form in a completely mass-segregated way?

Author(s): Pavlik, V (Pavlik, Vaclav); Kroupa, P (Kroupa, Pavel); Subr, L (Subr, Ladislav)

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 626 **Article Number:** A79 **DOI:** 10.1051/0004-6361/201834265 **Published:** JUN
Abstract: Context. ALMA observations of the Serpens South star-forming region suggest that stellar protoclusters may be compl birth. Independent observations also suggest that embedded clusters form segregated by mass.
Aims. As the primordial mass segregation seems to be lost over time, we aim to study on which timescale an initially perfectly m becomes indistinguishable from an initially not mass-segregated cluster. As an example, the Orion Nebula Cluster (ONC) is also
Methods. We used N-body simulations of star clusters with various masses and two different degrees of primordial mass segreg energy redistribution through two-body relaxation to quantify the time when the models agree in terms of mass segregation, w in the models that are primordially not mass segregated. A comprehensive cross-matched catalogue combining optical, infrare members was also compiled and made available.
Results. The models evolve to a similar radial distribution of high-mass stars after the core collapse (about half a median two-b become observationally indistinguishable from the point of view of mass segregation at time tau(v) approximate to 3.3 t(rh). In distribution of high-mass stars, we may not rule out either evolutionary scenario (regardless of whether they are initially mass s for extinction and elongation of the ONC, as reported elsewhere, an initially perfectly mass-segregated state seems to be more cluster.
Accession Number: WOS:000471755400003
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Pavlik, Vaclav	C-8848-2017	0000-0002-3031-062X

ISSN: 1432-0746

Record 98 of 235

Title: Experimental and theoretical investigation of solvatochromic properties and ion solvation structure in DESs of reline, glyc mixtures with PEG 400

Author(s): Aryafard, M (Aryafard, Meysam); Abbasi, M (Abbasi, Mostafa); Reha, D (Reha, David); Harifi-Mood, AR (Harifi-Mood, Ali Babak)

Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 284 **Pages:** 59-67 **DOI:** 10.1016/j.molliq.2019.03.149 **Published:** JUN 15 2
Abstract: Deep eutectic solvents (DESs) are a new class of ionic liquids which have been applied in many chemical reactions the their physicochemical properties such as hydrogen bond property and ion de localization, are important. We measured solvato different DESs, namely urea-choline chloride (reline), ethylene glycol-choline chloride (ethaline), and glycerol-choline chloride

mixtures with different mole fractions of poly ethylene glycol (PEG 400) as co-solvent. Solvatochromic results showed that the r in these three DESs, but the lowest in hydrogen bond donor and acceptor abilities. In binary mixtures of DESs with PEG 400, pi* decreasing with increasing the mole fraction of PEG 400 which is in good agreement with these parameters in mixed solvents. M confirmed that there are hydrogen bonds between urea, ethylene glycol, glycerol and choline chloride in pure DESs, and their a and also with some mole fractions of PEG 400. Moreover, delocalization of chloride in DESs, were calculated for all composition Also, MD simulations confirmed result of the experimental finding and preferential solvation model. (C) 2019 Elsevier B.V. All rig

Accession Number: WOS:000469154300008

Author Identifiers:

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ISSN: 0167-7322

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Record 99 of 235

Title: Interactions of star-like polyelectrolyte micelles with hydrophobic counterions

Author(s): Fernandez-Alvarez, R (Fernandez-Alvarez, Roberto); Nova, L (Nova, Lucie); Uhlik, F (Uhlik, Filip); Kereiche, S (Kereiche Mariusz); Kosovan, P (Kosovan, Peter); Matejicek, P (Matejicek, Pavel)

Source: JOURNAL OF COLLOID AND INTERFACE SCIENCE **Volume:** 546 **Pages:** 371-380 **DOI:** 10.1016/j.jcis.2019.03.054 **Publish**

Abstract: Hydrophobicity of a counterion has a profound effect on the interaction with polyelectrolytes similar to that of multiv understanding this interaction in weak polyelectrolyte micelles might assist in developing nanocarriers for pH-controlled encap We used star-like weak polyelectrolyte micelles of polystyrene-block-poly(2-vinyl pyridine) (PS-P2VP) with fixed aggregation nu polyelectrolyte, and cobalt bis(1,2-dicarbollide) (COSAN) as a model hydrophobic anion. We used NMR to assess the mobility of presence of varying amounts of COSAN, and at varying protonation degrees of the polyelectrolyte. Same experiments with indif used as a control. Furthermore, we used coarse-grained simulations to obtain a detailed picture of the effect of hydrophobic co conformation of the micelles.

A small amount of hydrophobic counterions causes morphological changes within the micelles, whereas a bigger amount caus confirmed both in simulations and in experiments. Furthermore, adsorption of the counterions induces ionization of the collap polyelectrolyte. Although the COSAN/P2VP system is rather specific, the generic model used in the coarse-grained simulations s behavior is a consequence of synergy of hydrophobic and electrostatic attraction between polyelectrolytes and hydrophobic cc general insights into the molecular mechanisms of these interactions. (C) 2019 Elsevier Inc. All rights reserved.

Accession Number: WOS:000466054200037

PubMed ID: 30933716

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Fernandez-Alvarez, Roberto	O-6043-2017	0000-0002-8914-9017

ISSN: 0021-9797

eISSN: 1095-7103

Record 100 of 235

Title: Chiroptical Redox Switching of Tetra-Cationic Derivatives of Azoniahelicenes

Author(s): Roncevic, I (Roncevic, Igor); Jirasek, M (Jirasek, Michael); Severa, L (Severa, Lukas); Reyes-Gutierrez, PE (Reyes-Gutie (Teply, Filip); Bednarova, L (Bednarova, Lucie); Hromadova, M (Hromadova, Magdalena); Pospisil, L (Pospisil, Lubomir)

Source: CHEMELECTROCHEM **Volume:** 6 **Issue:** 12 **Pages:** 3002-3008 **DOI:** 10.1002/celc.201900204 **Published:** JUN 14 2019

Abstract: New tetra- and di-cationic azoniahelicenes provide electrochemical, spectroelectrochemical and electronic circular d their differences in electron transfer (ET) kinetics. Di-cationic helquats containing two seven-membered rings are irreversibly re Substitution by redox-active ethenylpyridinium in the alpha or gamma position with respect to nitrogen atoms of the helquat c derivatives with reversible ET steps and communicating redox centres. Redox-inactive substituents in di-cationic azoniahelicen Redox switching of ECD of tetra-cationic enantiomers was observed. Unlike fully aromatic helquat, the ECD response of tetra-ca reduction-oxidation cycles is slower, owing to a strong adsorption on electrodes. Quantum chemical calculations (DFT) indicate cationic derivative substituted in the gamma position yields a folded structure, which favours the internal donor-acceptor inter

spectroelectrochemical differences between both tetra-cations.

Accession Number: WOS:000475465600004

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pospisil, Lubomir	F-5195-2014	
Bednarova, Lucie	E-7622-2012	
Gutierrez, Paul Eduardo Reyes	D-5606-2013	0000-0002-6325-8936
Hromadova, Magdalena	C-2369-2011	0000-0002-3138-6917

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Page 3 (Records 101 -- 150)
[1 | 2 | 3 | 4 | 5]

Record 101 of 235

Title: A semi-continuum model of saturation overshoot in one dimensional unsaturated porous media flow

Author(s): Kmec, J (Kmec, Jakub); Furst, T (Furst, Tomas); Vodak, R (Vodak, Rostislav); Sir, M (Sir, Miloslav)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 8390 **DOI:** 10.1038/s41598-019-44831-x **Published:** JUN 10 2019

Abstract: A semi-continuum model for fluid flow in saturated-unsaturated porous medium in one spatial dimension is presente well-established physics, measurable parameters and material characteristics. The porous material is characterized by porosity wetting and draining branches of the retention curve, and the saturation dependence of the relative permeability. The fluid is cl and dynamic viscosity. The only physics involved is the mass balance of fluid in porous media together with the Darcy-Buckingh unsaturated porous media. The model is a cellular automaton based on the Macro Modified Invasion Percolation concept of div blocks which are not infinitesimal and are assumed to retain the characteristics of a porous medium. The cellular automaton re saturation update in each block, pressure update in each block, and flux update between neighboring blocks. The model tracks saturation, the fluid capillary pressure, and the fluid flux. The model is shown to reproduce qualitatively and quantitatively all f saturation overshoot behavior reported in the literature.

Accession Number: WOS:000470847000014

PubMed ID: 31182825

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sir, Miloslav		0000-0002-6634-4071

ISSN: 2045-2322

Record 102 of 235

Title: DFT calculations reveal pronounced HOMO-LUMO spatial separation in polypyrrole-nanodiamond systems

Author(s): Matunova, P (Matunova, Petra); Jirasek, V (Jirasek, Vit); Rezek, B (Rezek, Bohuslav)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 21 **Issue:** 21 **Pages:** 11033-11042 **DOI:** 10.1039/c8cp07622g **Publis**

Abstract: The low-cost efficient generation of renewable energy and its blending with societal lifestyle is becoming increasingly inorganic-organic hybrid systems may have an immense, yet still mostly unexplored, potential in photovoltaic solar cells applic the interactions of polypyrrole (PPy) with diamond nanoparticles (so-called nanodiamonds, NDs) by computational density fun methods. We compute the structural and electronic properties of such hybrid organic-inorganic systems. During modeling, PPy physisorbed on (111) and (100) ND edge-like surface slabs terminated with oxygen, hydroxyl, carboxyl, and anhydride functiona arrangements most commonly found in real NDs. Moreover, NDs terminated with an amorphous surface layer (a-C: H, a-C: O) ar realistic conditions even further. In a predominant number of cases, we obtain the spatial separation of HOMO and LUMO at the dissociation. Further, there is a favorable energy level alignment for charge transport. The theoretical results, therefore, show tl ND composites in photovoltaic applications.

Accession Number: WOS:000471025900017

PubMed ID: 31089605

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rezek, Bohuslav	F-7403-2014	0000-0002-0378-4598

ISSN: 1463-9076

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Record 103 of 235

Title: Analysis of Long Molecular Dynamics Simulations Using Interactive Focus plus Context Visualization

Author(s): Byska, J (Byska, J.); Trautner, T (Trautner, T.); Marques, SM (Marques, S. M.); Damborsky, J (Damborsky, J.); Kozlikova (Waldner, M.)

Source: COMPUTER GRAPHICS FORUM **Volume:** 38 **Issue:** 3 **Pages:** 441-453 **DOI:** 10.1111/cgf.13701 **Published:** JUN 2019

Abstract: Analyzing molecular dynamics (MD) simulations is a key aspect to understand protein dynamics and function. With in power, it is now possible to generate very long and complex simulations, which are cumbersome to explore using traditional 3D movements. Guided by requirements derived from multiple focus groups with protein engineering experts, we designed and de

visual analysis approach for long and crowded MD simulations. In this approach, we link a dynamic 3D focus+context visualizati series data to guide the detection and navigation towards important spatio-temporal events. The 3D visualization renders elem and increases the temporal resolution dependent on the time series data or the spatial region of interest. In case studies with d sets and research questions, we found that the proposed visual analysis approach facilitates exploratory analysis to generate, c about causalities. Finally, we derived design guidelines for interactive visual analysis of complex MD simulation data.

Accession Number: WOS:000481468200035

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kozlikova, Barbora	G-3890-2014	
Marques, Sergio	H-8685-2012	0000-0002-6281-7505

ISSN: 0167-7055

eISSN: 1467-8659

Record 104 of 235

Title: Toward Accurate Hydrogen Bonds by Scalable Quantum Monte Carlo

Author(s): Dubecky, M (Dubecky, Matus); Jurecka, P (Jurecka, Petr); Mitas, L (Mitas, Lubos); Ditte, M (Ditte, Matej); Fanta, R (Fant

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 15 **Issue:** 6 **Pages:** 3552-3557 **DOI:** 10.1021/acs.jctc.9b0

Abstract: Single-determinant (SD) fixed-node diffusion Monte Carlo (FNDMC) gains popularity as a benchmark method scalable systems, although its accuracy limits are not yet fully mapped out. We report on an interesting example of significant SD FNDMC middle-sized hydrogen-bonded dimer complexes, formic acid (FA) vs methanediol (MD), distinct by the maximum bond order (2 SD FNDMC schemes based on bias cancellation are capable of achieving benchmark (2%) accuracy for MD, this has not been the leading systematic error source in energy differences and show that suitably designed Jastrow factors enable SD FNDMC to reac FA. This work clearly illustrates the varying accuracy of the present-day SD FNDMC at the 0.1 kcal/mol scale for a particular set c promising routes toward alleviation of these shortcomings, still within the single-reference framework.

Accession Number: WOS:000471728500011

PubMed ID: 31026158

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Dubecky, Matus	P-1720-2016	

ISSN: 1549-9618

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Record 105 of 235

Title: Redox properties and human serum albumin binding of nitro-oleic acid

Author(s): Zatloukalova, M (Zatloukalova, Martina); Mojovic, M (Mojovic, Milos); Pavicevic, A (Pavicevic, Aleksandra); Kabelac, M BA (Freeman, Bruce A.); Pekarova, M (Pekarova, Michaela); Vacek, J (Vacek, Jan)

Source: REDOX BIOLOGY **Volume:** 24 **Article Number:** UNSP 101213 **DOI:** 10.1016/j.redox.2019.101213 **Published:** JUN 2019

Abstract: Nitro-fatty acids modulate inflammatory and metabolic stress responses, thus displaying potential as new drug candi the redox behavior of nitro-oleic acid (NO2-OA) and its ability to bind to the fatty acid transporter human serum albumin (HSA). underwent electrochemical reduction at - 0.75 V at pH 7.4 in an aqueous milieu. Based on observations of the R-NO2 reduction reactivity of NO2-OA was measured in comparison to oleic acid (OA) as the negative control. These electrochemically-based res computational quantum mechanical modeling. DFT calculations indicated that both the C9-NO2 and C10-NO2 positional isome conformers with different internal angles (69 degrees and 110 degrees) between the methyl- and carboxylate termini. Both NO2 LUMO energies of around - 0.7 eV, affirming the electrophilic properties of fatty acid nitroalkenes. In addition, the binding of NO revealed a molar ratio of similar to 7:1 [NO2-OA]: [HSA]. These binding experiments were performed using both an electrocataly paramagnetic resonance (EPR) spectroscopy using 16-doxyl stearic acid. Using a Fe(DTCS)(2) spin-trap, EPR studies also showec moiety of NO2 -OA resulted in the formation of nitric oxide radical. Finally, the interaction of NO2-OA with HSA was monitored v oxidation. The results indicate that not only non-covalent binding but also NO2-OA-HSA adduction mechanisms should be take study of the redox properties of NO2-OA is applicable to the characterization of other electrophilic mediators of biological and p

Accession Number: WOS:000471255400042

PubMed ID: 31170679

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 2213-2317

Record 106 of 235

Title: Activation of innate immunity by mitochondrial dsRNA in mouse cells lacking p53 protein

Author(s): Wiatrek, DM (Wiatrek, Dagmara M.); Candela, ME (Candela, Maria E.); Sedmik, JI (Sedmik, Jiri I.); Oppelt, J (Oppelt, Ja P.); O'Connell, MA (O'Connell, Mary A.)

Source: RNA **Volume:** 25 **Issue:** 6 **Pages:** 713-726 **DOI:** 10.1261/rna.069625.118 **Published:** JUN 2019

Abstract: Viral and cellular double-stranded RNA (dsRNA) is recognized by cytosolic innate immune sensors, including RIG-I-like dsRNA is commonly present in cells, and one source is mitochondrial dsRNA, which results from bidirectional transcription of m Here we demonstrate that Trp53 mutant mouse embryonic fibroblasts contain immune-stimulating endogenous dsRNA of mito that the immune response induced by this dsRNA is mediated via RIG-I-like receptors and leads to the expression of type I interf cytokine genes. The mitochondrial dsRNA is cleaved by RNase L, which cleaves all cellular RNA including mitochondrial mRNAs I-like receptors. When mitochondrial transcription is interrupted there is a subsequent decrease in this immune-stimulatory dsR the role of p53 in innate immunity is even more versatile and complex than previously anticipated. Our study, therefore, sheds r endogenous RNA in diseases featuring aberrant immune responses.

Accession Number: WOS:000468092200005

PubMed ID: 30894411

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
O'Connell, Mary Anne	G-4740-2015	0000-0003-3844-6174

ISSN: 1355-8382

eISSN: 1469-9001

Record 107 of 235

Title: Identification and classification of DICOM files with burned-in text content

Author(s): Vcelak, P (Vcelak, Petr); Kryl, M (Kryl, Martin); Kratochvil, M (Kratochvil, Michal); Kleckova, J (Kleckova, Jana)

Source: INTERNATIONAL JOURNAL OF MEDICAL INFORMATICS **Volume:** 126 **Pages:** 128-137 **DOI:** 10.1016/j.ijmedinf.2019.02.01

Abstract: Background: Protected health information burned in pixel data is not indicated for various reasons in DICOM. It compl such data. In recent years, there have been several attempts to anonymize or de-identify DICOM files. Existing approaches have completely reliable solution exists. Especially for large datasets, it is necessary to quickly analyse and identify files potentially v Methods: Classification is based on adaptive-iterative algorithm designed to identify one of three classes. There are several ima character recognition, and filters; then a local decision is made. A confirmed local decision is the final one. The classifier was tra of 15,334 images of various modalities.

Results: The false positive rates are in all cases below 4.00%, and 1.81% in the mission-critical problem of detecting protected h classifier's weighted average recall was 94.85%, the weighted average inverse recall was 97.42% and Cohen's Kappa coefficient Conclusion: The proposed novel approach for classification of burned-in text is highly configurable and able to analyse images a noisy background. The solution was validated and is intended to identify DICOM files that need to have restricted access or be to privacy issues. Unlike with existing tools, the recognised text, including its coordinates, can be further used for de-identificati

Accession Number: WOS:000465414600016

PubMed ID: 31029254

ISSN: 1386-5056

eISSN: 1872-8243

Record 108 of 235

Title: Examining PBKDF2 security margin-Case study of LUKS

Author(s): Visconti, A (Visconti, Andrea); Mosnacek, O (Mosnacek, Ondrej); Broz, M (Broz, Milan); Matyas, V (Matyas, Vashek)

Source: JOURNAL OF INFORMATION SECURITY AND APPLICATIONS **Volume:** 46 **Pages:** 296-306 **DOI:** 10.1016/j.jisa.2019.03.016

Abstract: Passwords are widely used to protect our sensitive information or to gain access to specific resources. They should be strong enough to prevent well-known attacks. Unfortunately, user-chosen passwords are usually short and lack sufficient entro these problems is to adopt a Key Derivation Function (KDF) that allows legitimate users to spend a moderate amount of time or imposing CPU/memory-intensive operations on the attacker side. In this paper, we focus on long-term passwords secured by th

Derivation Function 2 (PBKDF2) and present the case study of Linux Unified Key Setup (LUKS), a disk-encryption specification c Linux based operating systems. In particular, we describe how LUKS protects long-term keys by means of iteration counts defin how external factors may affect the iteration counts computation. In doing so, we provide means of evaluating the iteration cou and experimentally show to what level PBKDF2 is still capable of providing sufficient security margin for a LUKS implementatio rights reserved.

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Record 109 of 235

Title: Temperature-dependent resistivity and anomalous Hall effect in NiMnSb from first principles

Author(s): Wagenknecht, D (Wagenknecht, David); Smejkal, L (Smejkal, Libor); Kaspar, Z (Kaspar, Zdenek); Sinova, J (Sinova, Ja Tomas); Kudrnovsky, J (Kudrnovsky, Josef); Carva, K (Carva, Karel); Turek, I (Turek, Ilja)

Source: PHYSICAL REVIEW B **Volume:** 99 **Issue:** 17 **Article Number:** 174433 **DOI:** 10.1103/PhysRevB.99.174433 **Published:** MA

Abstract: We present implementation of the alloy analogy model within fully relativistic density-functional theory with the coh for a treatment of nonzero temperatures. We calculate contributions of phonons and magnetic and chemical disorder to the ter resistivity, anomalous Hall conductivity (AHC), and spin-resolved conductivity in ferromagnetic half-Heusler NiMnSb. Our electr with combined scattering effects agree well with experimental literature for Ni-rich NiMnSb with 1-2% Ni impurities on Mn subla dominated by the Fermi surface term in the Kubo-Bastin formula. Moreover, the AHC as a function of longitudinal conductivity the Ni-rich alloy, while it is nonmonotonic for Mn impurities. We obtain the spin polarization of the electrical current P > 90% at show that P may be tuned by chemical composition. The presented results demonstrate the applicability of an efficient first-pri temperature dependence of linear transport coefficients in multisublattice bulk magnetic alloys.

Accession Number: WOS:000469324500007

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Jungwirth, Tomas	G-8952-2014	0000-0002-9910-1674
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Wagenknecht, David	P-4165-2017	0000-0003-1927-9702

ISSN: 2469-9950

eISSN: 2469-9969

Record 110 of 235

Title: Structural interpretation of the P-31 NMR chemical shifts in thiophosphate and phosphate: key effects due to spin-orbit ar

Author(s): Fukal, J (Fukal, J.); Pav, O (Pav, O.); Budesinsky, M (Budesinsky, M.); Rosenberg, I (Rosenberg, I.); Sebera, J (Sebera, J. V.)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 21 **Issue:** 19 **Pages:** 9924-9934 **DOI:** 10.1039/c9cp01460h **Publishe**

Abstract: Structural interpretation of the P-31 NMR shifts measured in O,O-diethyl thiophosphate (PT), 5,5-dimethyl-2- mercapt 2-oxide (cPT), diethylphosphate (P) and 5,5-dimethyl-2-hydroxy-1,3,2-dioxaphosphinane 2-oxide (cP) was obtained by means o including the effects of geometry, molecular dynamics, and solvent, relativistic effects and the effect of NMR reference. NMR cal B3LYP, BP86, BPW91, M06-2X, PBE0, MP2, and HF methods, the Iglo-n (n = II, III), cc-pVnZ (n = D, T, Q, 5), and pcS-n (n = 0, 1, 2, 3, and the Slatertype QZ4P atomic basis. Water solvent was described explicitly and/or implicitly. The effects due to molecular dy molecular dynamics simulations with the GAFF force field and the TIP3P water molecules, and alternatively by means of the zer averaging. Relativistic effects included the spin-orbit calculated within the two-component zero-order relativistic approximatio component DFT method. Optimal geometries and largeamplitude dynamical motions within the "opened" PT and P molecules different geometries and confined dynamical motions within the cPT and cP "closed" molecules. These structuredynamical diff different chemical structures of thiophosphate and phosphate due to a non-esterified sulphur or oxygen atom within the group magnitudes of P-31 NMR shifts. The theoretical calculations enabled accurate and reliable structure-dynamical interpretation o shifts. The effects due to explicit solvent and relativity turned out to be indispensable for obtaining accurate P-31 NMR shifts pa thiophosphates. Replacement of the non-esterified oxygen atom in the phosphate with sulphur makes NMR shielding of the ph different as compared to the NMR shielding of the phosphorus atom in phosphate, H3PO4 and PH3.

Accession Number: WOS:000473071200027

PubMed ID: 31038518

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Fukal, Jiri	S-7922-2017	0000-0002-0188-8828
Sebera, Jakub	B-6112-2013	0000-0001-5671-5206

ISSN: 1463-9076

eISSN: 1463-9084

Record 111 of 235

Title: Experimental and theoretical study of propene adsorption on alkali metal exchanged FER zeolites

Author(s): Bulanek, R (Bulanek, Roman); Koudelkova, E (Koudelkova, Eva); Ramos, FSD (Ramos, Francisca Solanea de Oliveira); Bludsky, O (Bludsky, Ota); Rubes, M (Rubes, Miroslav); Cejka, J (Cejka, Jiri)

Source: MICROPOROUS AND MESOPOROUS MATERIALS **Volume:** 280 **Pages:** 203-210 **DOI:** 10.1016/j.micromeso.2019.02.003 **P**

Abstract: Propene adsorption on Li- and Na-FER zeolites was investigated combining IR spectroscopy and calorimetric measure with DFT calculations using a DFT/CC scheme based on the PBE density functional. Considering the good agreement between e results, the following adsorption complexes of propene in the M-FER zeolites investigated in this study can be distinguished: (i) zeolitic framework via dispersion interactions mainly populated in zeolites with a high Si/Al ratio and with a characteristic nu(C= cm(-1) and adsorption heat of approximately 48 kJ/mol, (ii) propene interacting with cations coordinated in 6-rings characterize (Li-FER) and 1636 cm(-1) (Na-FER), (iii) propene adsorbed on remaining cationic positions excluding cationic positions in 6-rings 1630 cm(-1) (Li-FER) and 1633 cm(-1) (Na-FER) and (iv) propene bridging two nearby sodium cations in dual-cation sites charact at 1626 cm(-1) and with an adsorption heat of 85 kJ/mol, which is 6 kJ/mol higher than that of the strongest interaction with a s The population of bridged complexes in Na-FER was significantly lower than those in previously studied K-FER zeolites due to th cations for 8-rings, which is more suitable for the creation of dual-cation sites than 6-rings, wherein sodium cations are preferer bridged complexes were found in the case of Li-FER because Li+ cations are closer to the framework oxygen atoms and thus rela each other.

Accession Number: WOS:000462419400024

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Cejka, Jiri	AAC-6209-2019	
Trachta, Michal	G-8118-2014	0000-0001-5084-3434

ISSN: 1387-1811

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Record 112 of 235

Title: Diketopyrrolopyrrole-Based Organic Solar Cells Functionality: The Role of Orbital Energy and Crystallinity

Author(s): Heinrichova, P (Heinrichova, Patricie); Pospisil, J (Pospisil, Jan); Stritesky, S (Stritesky, Stanislav); Vala, M (Vala, Marti Toman, P (Toman, Petr); Rais, D (Rais, David); Pfleger, J (Pfleger, Jiri); Vondracek, M (Vondracek, Martin); Simek, D (Simek, Danie Horakova, P (Horakova, Petra); Dokladalova, L (Dokladalova, Lenka); Kubac, L (Kubac, Lubomir); Kratochvilova, I (Kratochvilova

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 123 **Issue:** 18 **Pages:** 11447-11463 **DOI:** 10.1021/acs.jpcc.9b01328 **Pub**

Abstract: In this work, we investigated diketopyrrolopyrrole (DPP) derivatives as potential donor materials for fullerene:DPP sol bis(5-(benzofuran-2-yOthiophene-2-yl)-2,5-bis(2-ethylhexyl)pyrrolo [3,4-c]-pyrrole-1,4-dione (DPP(TBFu)(2)) and 3,6-bis(5-(ben 2-yl)-2,5-bis(2-ethylhexyl)pyrrolo [3,4-c]-pyrrole-1,4-dione (DPP(TBTh)(2)) were modified by introducing a nitrogen atom into th molecule. Our quantum -chemical calculations predicted that this modification would increase the rigidity of the molecular stru ionization potential relative to the original DPP derivatives. The higher ionization potential primarily supports an enhancement and a more rigid molecular structure will contribute to reduced nonradiative losses. We experimentally verified the fullerene:DP the coincidence of a smaller driving force for charge separation at the donor/acceptor interface and the crystallinity of the studi preparing effective photovoltaic devices. The reduction of the driving force for charge separation could be overcome by more st materials; the delocalization of electrons and holes in such structured materials improves charge separation in OPV devices. Us experimental methods, we determined the parameters of the studied DPP materials with PC70BM in thin films. This work contri applications by verifying the concept of this organic solar cell design.

Accession Number: WOS:000467781000014

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rais, David	G-6682-2014	

Pfleger, Jiri	A-2965-2014	0000-0001-9576-7551
Kratochvilova, I.	G-5571-2014	0000-0002-6633-9432
Fekete, Ladislav	F-7498-2011	0000-0002-8548-2613
Vala, Martin	A-1489-2009	0000-0003-2229-6669
Toman, Petr	B-1834-2009	
Vondracek, Martin	E-5448-2013	0000-0003-4150-139X
Toman, Petr		0000-0002-1607-0332

ISSN: 1932-7447

Record 113 of 235

Title: Modeling of interactions between supernovae ejecta and aspherical circumstellar environments

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

Source: ASTRONOMY & ASTROPHYSICS **Volume:** 625 **Article Number:** A24 **DOI:** 10.1051/0004-6361/201833429 **Published:** MA

Abstract: Context. Massive stars are characterized by a significant loss of mass either via (nearly) spherically symmetric stellar w or by aspherical forms of circumstellar matter (CSM) such as bipolar lobes or outflowing circumstellar equatorial disks. Since a s massive stars end their lives by a core collapse, supernovae (SNe) are always located inside large circumstellar envelopes create Aims. We study the dynamics and thermal effects of collision between expanding ejecta of SNe and CSM that may be formed du star phase, a luminous blue variable phase, around PopIII stars, or by various forms of accretion.

Methods. For time-dependent hydrodynamic modeling we used our own grid-based Eulerian multidimensional hydrodynamic volumes method. The code is based on a directionally unsplit Roe's method that is highly efficient for calculations of shocks an discontinuities.

Results. We simulate a SNe explosion as a spherically symmetric blast wave. The initial geometry of the disks corresponds to a d that orbits in Keplerian trajectories. We examine the behavior of basic hydrodynamic characteristics, i.e., the density, pressure, temperature structure in the interaction zone under various geometrical configurations and various initial densities of CSM. We SN-CSM system and the rate of aspherical deceleration as well as the degree of anisotropy in density, pressure, and temperatur Conclusions. Our simulations reveal significant asphericity of the expanding envelope above all in the case of dense equatorial model however also shows significant asphericity in the case of the disk mass-loss rate (M)over dot(csd)= 10(-6)M(circle dot) yr(zones of overdensity in the SN-disk contact region and indicate the development of Kelvin-Helmholtz instabilities within the zo and the more freely expanding material outside the disk.

Accession Number: WOS:000466697700002

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kurfurst, Petr	X-7734-2019	

ISSN: 1432-0746

Record 114 of 235

Title: The influence of distributed source regions in the formation of the nonlinear distortion component of cubic distortion-pro

Author(s): Vencovsky, V (Vencovsky, Vaclav); Zelle, D (Zelle, Dennis); Dalhoff, E (Dalhoff, Ernst); Gummer, AW (Gummer, Anthony Ales)

Source: JOURNAL OF THE ACOUSTICAL SOCIETY OF AMERICA **Volume:** 145 **Issue:** 5 **Pages:** 2909-2931 **DOI:** 10.1121/1.5100611

Abstract: Distortion product otoacoustic emissions (DPOAEs) are evoked by two stimulus tones with frequency f(1) and f(2) of r between approximately 1.05 and 1.4. This study theoretically and experimentally analyzes the cubic 2f(1) - f(2) DPOAE for differe the tones while the other is constant. Simulations for f(2)/f(1) of 1.2 and moderate stimulus levels (30-70 dB sound pressure lev distortion products are generated along a relatively large length of the basilar membrane, the extent of which increases with sti from the place of maximum nonlinear force, the wavelets generated by these distributed sources mutually cancel. Therefore, al the primary DPOAE sources broadens with increasing stimulus level (up to 1.5 oct), the basilar-membrane region contributing t relatively narrow (0.6 oct) and level independent. The observed dependence of DPOAE amplitude on stimulus level can be well source at the basilar-membrane place where the largest distortion product (maximum of the nonlinear force) is generated. Ons signal may contain amplitude overshoots (complexities), which are in most cases asymmetrical. Two-tone suppression was ide these onset and offset complexities. DPOAE measurements in two normal-hearing subjects support the level dependence of the amplitude and the asymmetry in the onset and offset responses predicted by the theoretical analysis. (C) 2019 Acoustical Socie

Accession Number: WOS:000483973600027

PubMed ID: 31153314

ISSN: 0001-4966

eISSN: 1520-8524

Record 115 of 235

Title: High-throughput small RNA sequencing for evaluation of grapevine sanitation efficacy

Author(s): Eichmeier, A (Eichmeier, Ales); Kominkova, M (Kominkova, Marcela); Pecenka, J (Pecenka, Jakub); Kominek, P (Komi

Source: JOURNAL OF VIROLOGICAL METHODS **Volume:** 267 **Pages:** 66-70 **DOI:** 10.1016/j.jviromet.2019.03.003 **Published:** MAY

Abstract: This study describes the application of high-throughput sequencing of small RNA analysis of the efficacy of using Riba leafroll-associated virus 1, Grapevine fleck virus and Grapevine rupestris stem pitting-associated virus from Vitis vinifera cv. Ries for sanitation by Ribavirin treatment was one naturally infected with all the viruses mentioned above as confirmed by RT-PCR. A were established and plantlets obtained were sanitized using Ribavirin. Three years after sanitation, a small RNA sequencing m targeting 21, 22 and 24 nt-long viral small RNAs (vsRNAs), was used to analyze both the mother plant and the sanitized plants. T mother plant was infected by the three mentioned viruses and additionally by two viroids - Hop stunt viroid and Grapevine yell Ribavirin treatment, the plants contained only the two viroids, with the complete elimination of all the viruses previously prese

Accession Number: WOS:000465365600011

PubMed ID: 30851291

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Eichmeier, Ales	Q-4622-2019	
Kominek, Petr	AAD-1578-2019	
Eichmeier, Ales		0000-0001-7358-3903
Pecenka, Jakub		0000-0001-6195-7592

ISSN: 0166-0934

eISSN: 1879-0984

Record 116 of 235

Title: A general hydrogen bonding definition based on three-dimensional spatial distribution functions and its extension to qua solutions and general intermolecular bonds

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

Source: JOURNAL OF MOLECULAR LIQUIDS **Volume:** 281 **Pages:** 225-235 **DOI:** 10.1016/j.molliq.2019.02.036 **Published:** MAY 1

Abstract: Numerous microscopic definitions of hydrogen bonding have been proposed and employed in molecular simulations various energetic, topological, and geometric criteria and require a specification of the cut-off values. The cut-off values are cho description of hydrogen bonding in a particular molecular system under particular conditions and for a particular molecular m straightforwardly transferable to different molecular systems or conditions. We propose a general approach to define and quan in liquids and solutions, including hydrogen bonds, which is free of any cutoff values. The approach is based on finding a contin surroundings of a local maximum of a spatial distribution function, enclosed by an isosur-face going through the nearest signifi the general definition of intermolecular bonding can quantify significance of particular intermolecular bonds or can be used loc characterise bonds in heterogeneous systems or confinement. Besides the general definition of the intermolecular bonding, the characterised by a number of relevant properties such as the number of bonds per molecule, volume of a bond region per mole or hydration number to provide deep insight into the intermolecular bonding. The approach is demonstrated for pure water an under different thermodynamic conditions, and our results on the behaviour and quantification of their intermolecular bondin obtained using commonly-used bond definitions. (C) 2019 Elsevier B.V. All rights reserved.

Accession Number: WOS:000465049400025

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Author	Web of Science ResearcherID	ORCID Number
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Svoboda, Martin	L-9724-2015	0000-0002-8449-2078

ISSN: 0167-7322

eISSN: 1873-3166

Record 117 of 235

Title: Correlating structural and mechanical properties of AlN/TiN superlattice films

Author(s): Koutna, N (Koutna, Nikola); Rehak, P (Rehak, Petr); Chen, Z (Chen, Zhuo); Bartosik, M (Bartosik, Matthias); Fallmann, M (Cerny, Miroslav); Zhang, Z (Zhang, Zaoli); Friak, M (Friak, Martin); Sob, M (Sob, Mojmir); Mayrhofer, PH (Mayrhofer, Paul H.); H

Source: SCRIPTA MATERIALIA **Volume:** 165 **Pages:** 159-163 **DOI:** 10.1016/j.scriptamat.2019.02.021 **Published:** MAY 2019

Abstract: Combining first-principles and experimental techniques, we establish Young's modulus dependence of AlN/TiN super phases, their thicknesses and crystallographic orientations. The disparate character of cleavage properties within different laye providing indications regarding crack initiation processes-is linked to the changes in bond lengths. Such changes present a dire predicted interplanar spacing oscillations which are experimentally confirmed by high resolution transmission electron micros

Accession Number: WOS:000463127300033

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Bartosik, Matthias		0000-0001-5398-4304
Sob, Mojmir	G-6865-2011	0000-0002-5724-890X

ISSN: 1359-6462

Record 118 of 235

Title: Theoretical investigations on structural, elastic, thermodynamic and electronic properties of Al3Ti and Al3V compounds i pressure

Author(s): Meng, FS (Meng, Fan-Shun); Yao, Z (Yao, Zhen); Vsianskaa, M (Vsianska, Monika); Friaak, M (Friak, Martin); Sob, M (Sob

Source: MATERIALS RESEARCH EXPRESS **Volume:** 6 **Issue:** 5 **Article Number:** 056536 **DOI:** 10.1088/2053-1591/aafec0 **Publishe**

Abstract: The structural, mechanical, thermodynamic and electronic properties of intermetallic compounds Al3Ti and Al3V in L range of 0-100 GPa have been investigated using first-principles method. The calculated structural parameters and energy infor are consistent with the available experimental and theoretical results. The stability of Al3Ti and Al3V in L1(2) structure is checke phonon calculation. The values of bulk modulus, shear modulus, Young's modulus, hardness, Poisson ratio, anisotropy index, D velocities increase with the increasing external pressure. The compound Al3V in L1(2)structure possesses interesting properties pressure region (up to 20 GPa) but weakly brittle behavior at high pressures (above 30 GPa) and the minimum value of Poisson r pressure. Finally, the pressure-dependence behavior of density of states and charge densities are analyzed to explore the bond origin of the pressure effect on the various properties of Al3Ti and Al3V.

Accession Number: WOS:000459152200001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sob, Mojmir	G-6865-2011	0000-0002-5724-890X
Vsianska, Monika	O-7454-2015	

ISSN: 2053-1591

Record 119 of 235

Title: Practical Guide to Quantum Phase Transitions in Quantum-Dot-Based Tunable Josephson Junctions

Author(s): Kadlecova, A (Kadlecova, A.); Zonda, M (Zonda, M.); Pokorny, V (Pokorny, V.); Novotny, T (Novotny, T.)

Source: PHYSICAL REVIEW APPLIED **Volume:** 11 **Issue:** 4 **Article Number:** 044094 **DOI:** 10.1103/PhysRevApplied.11.044094 **Pu**

Abstract: Quantum dots attached to BCS superconducting leads exhibit a 0 - pi impurity quantum phase transition, which can b either by the gate voltage or by the superconducting phase difference. For the pertinent superconducting single-impurity Ande simple analytical formulae describing the position of the phase boundary in parameter space for the weakly correlated and Kor Furthermore, we show that the two-level approximation provides an excellent description of the low-temperature physics of su near the phase transition. We discuss reliability and mutual agreement of available finite-temperature numerical methods (nun and quantum Monte Carlo) and suggest an alternative approach for efficient determination of the quantum phase boundary fro temperature data. Our results enable fast and efficient, yet reliable characterization and design of such nanoscopic tunable Jos

Accession Number: WOS:000466447500003

Author Identifiers:

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

ISSN: 2331-7019

Record 120 of 235

Title: Molecular polarizability in open ensemble simulations of aqueous nanoconfinements under electric field

Author(s): Moucka, F (Moucka, F.); Zamfir, S (Zamfir, S.); Bratko, D (Bratko, D.); Luzar, A (Luzar, A.)

Source: JOURNAL OF CHEMICAL PHYSICS **Volume:** 150 **Issue:** 16 **Article Number:** 164702 **DOI:** 10.1063/1.5094170 **Published:**

Abstract: Molecular polarization at aqueous interfaces involves fast degrees of freedom that are often averaged out in atomistic resulting effective interactions depend on a specific environment, making explicit account of molecular polarizability particular pronounced anisotropic perturbations, including solid/liquid interfaces and external fields. Our work concerns polarizability eff confinements under electric field, open to an unperturbed bulk environment. We model aqueous molecules and ions in hydrop Gaussian-charge-on-spring BK3-AH representation. This involves nontrivial methodology developments in expanded ensemble open systems with long-ranged multibody interactions and necessitates further improvements for efficient modeling of polariz differences between fixed chargeand polarizable models were captured in molecular dynamics simulations for a set of closed s results with the BK3 model in neat aqueous systems capture the 10% reduction of molecular dipoles within the surface layer ne walls in analogy to reported quantum mechanical calculations at water/vapor interfaces. The polarizability affects the interfaci weakens the electric-field dependence of water absorption at pragmatically relevant porosities. We observe moderate changes and atom and charged-site spatial distributions; the Gaussian distribution of mobile charges on water and ions in the polarizab amplitudes and blurs the charge-layering effects associated with increased ion absorption. The use of polarizable force field inc of interfacial ion distributions to applied electric field, a feature potentially important for in silk() modeling of electric double la

Accession Number: WOS:000466698700047

PubMed ID: 31042910

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 0021-9606

eISSN: 1089-7690

Record 121 of 235

Title: Interactions between cyclic nucleotides and common cations: an ab initio molecular dynamics study

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

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 21 **Issue:** 15 **Pages:** 8121-8132 **DOI:** 10.1039/c8cp07492e **Publishe**

Abstract: We present the first, to the best of our knowledge, ab initio molecular dynamics (AIMD) investigation on three aqueou cyclic nucleotide model is solvated in the presence of distinct cations (i.e., Na+, K+ and Mg2+). We elucidate the typical modaliti those ionic species and the nucleotide moiety by first-principles numerical simulations, starting from an inner-shell binding cor 100 ps (total simulation time of approximate to 600 ps). Whereas the strong structure-maker Mg2+ is permanently bound to one the phosphate group of the nucleotide model, Na+ and K+ show binding times (b) of 65 ps and 10-15 ps, respectively, thus refle aqueous solutions. Furthermore, we qualitatively relate these findings to approximate free-energy barriers of the cations' unbir exploratory well-tempered metadynamics. With the aim of shedding light on the features of commonly employed force-fields (F (almost 200 trajectories with a total simulation time of approximate to 18 s) using the biomolecular AMBER FF are also reported combinations of the parametrization for the water environment (i.e., TIP3P, SPC/E and OPC) and cations (i.e., Joung-Cheatham, 12-6-4), we found significant differences in the radial distribution functions and residence times compared to the ab initio resul wrongly show quasi-identical radial distribution functions and the Li & Merz 12-6-4 Lennard-Jones parameters for Mg2+ were fo reaching the binding state consistent with AIMD.

Accession Number: WOS:000465260400041

PubMed ID: 30932112

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Cassone, Giuseppe	M-8290-2015	0000-0003-1895-2950

ISSN: 1463-9076

eISSN: 1463-9084

Record 122 of 235

Title: Microfriction correction factor to the Stokes-Einstein equation for small molecules determined by NMR diffusion measure modelling

Author(s): Dvorak, P (Dvorak, Petr); Soltesova, M (Soltesova, Maria); Lang, J (Lang, Jan)

Source: MOLECULAR PHYSICS **Volume:** 117 **Issue:** 7-8 **Special Issue:** SI **Pages:** 868-876 **DOI:** 10.1080/00268976.2018.1510144

Abstract: The Stokes-Einstein relationship relating the self-diffusion coefficient with the size of a diffusing particle (a hydrodyna case of small molecules. We present a novel method extending the range of validity of the Stokes-Einstein relationship by mean specific microfriction correction factor. This factor equals to 1 in the ordinary form of the Stokes-Einstein formula for stick' bour molecules of solvent are much smaller than the diffusing particle. We have determined the microfriction correction factors for s (ranging in size from ethanol to 18-crown-6 ether and tetrakis(trimethylsilyl)silane) in a dilute hexane solution by a concerted u measurements and the molecular hydrodynamic calculations. Both of the tested hydrodynamic modelling programmes, Hydro J. Magn. Reson. 2000, 147, 138-146) and DiTe (Barone et al., J. Comput. Chem. 2008, 30, 2-13) provided very similar results after molecular system, which is within the validity range of the Stokes-Einstein relationship (fullerene in hexane solution in this wor

Accession Number: WOS:000474854300006

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Soltesova, Maria	U-5856-2017	0000-0003-3579-590X
Dvorak, Petr	C-6441-2017	0000-0002-7839-8587

ISSN: 0026-8976

eISSN: 1362-3028

Record 123 of 235

Title: Anncolvar: Approximation of Complex Collective Variables by Artificial Neural Networks for Analysis and Biasing of Molecu

Author(s): Trapl, D (Trapl, Dalibor); Horvacanin, I (Horvacanin, Izabela); Mareska, V (Mareska, Vaclav); Ozcelik, F (Ozcelik, Furkar Spiwok, V (Spiwok, Vojtech)

Source: FRONTIERS IN MOLECULAR BIOSCIENCES **Volume:** 6 **Article Number:** UNSP 25 **DOI:** 10.3389/fmolb.2019.00025 **Publis**

Abstract: The state of a molecular system can be described in terms of collective variables. These low-dimensional descriptors used to monitor the state of the simulation, to calculate free energy profiles or to accelerate rare events by a bias potential or a calculation of some complex collective variables may slow down the simulation or analysis of trajectories. Moreover, many colle explicitly calculated for newly sampled structures. In order to address this problem, we developed a new package called annco possible to build and train an artificial neural network model that approximates a collective variable. It can be used to generate enhanced sampling simulation PLUMED package, so the collective variable can be monitored and biased by methods available computational efficiency and the accuracy of anncolvar are demonstrated on selected molecular systems (cyclooctane derivati selected collective variables (Isomap, molecular surface area).

Accession Number: WOS:000466810700002

PubMed ID: 31058167

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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eISSN: 2296-889X

Record 124 of 235

Title: Dishevelled-3 conformation dynamics analyzed by FRET-based biosensors reveals a key role of casein kinase 1

Author(s): Harnos, J (Harnos, Jakub); Canizal, MCA (Canizal, Maria Consuelo Alonso); Jurasek, M (Jurasek, Miroslav); Kumar, J (I (Holler, Cornelia); Schambony, A (Schambony, Alexandra); Hanakova, K (Hanakova, Katerina); Bernatik, O (Bernatik, Ondrej); Zc Gomoryova, K (Gomoryova, Kristina); Gybel, T (Gybel, Tomas); Radaszkiewicz, TW (Radaszkiewicz, Tomasz Witold); Kravec, M (K (Trantirek, Lukas); Rynes, J (Rynes, Jan); Dave, Z (Dave, Zankruti); Fernandez-Llamazares, AI (Fernandez-Llamazares, Ana Iris); V Tripsianes, K (Tripsianes, Konstantinos); Hoffmann, C (Hoffmann, Carsten); Bryja, V (Bryja, Vitezslav)

Source: NATURE COMMUNICATIONS **Volume:** 10 **Article Number:** 1804 **DOI:** 10.1038/s41467-019-09651-7 **Published:** APR 18 2

Abstract: Dishevelled (DVL) is the key component of the Wnt signaling pathway. Currently, DVL conformational dynamics under unknown. To overcome this limitation, we develop the Fluorescein Arsenical Hairpin Binder- (FlAsH-) based FRET in vivo approa in living cells. Using this single-cell FRET approach, we demonstrate that (i) Wnt ligands induce open DVL conformation, (ii) DVL predominantly open, show more even subcellular localization and more efficient membrane recruitment by Frizzled (FZD) and (CK1 epsilon) has a key regulatory function in DVL conformational dynamics. In silico modeling and in vitro biophysical method specific phosphorylation events control DVL conformations via modulation of the PDZ domain and its interaction with DVL C-te study describes an experimental tool for DVL conformational sampling in living cells and elucidates the essential regulatory rol conformational dynamics.

Accession Number: WOS:000464979000002

PubMed ID: 31000703

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 2041-1723

Record 125 of 235

Title: EEG spatiospectral patterns and their link to fMRI BOLD signal via variable hemodynamic response functions

Author(s): Labounek, R (Labounek, Rene); Bridwell, DA (Bridwell, David A.); Marecek, R (Marecek, Radek); Lamos, M (Lamos, Ma Bednarik, P (Bednarik, Petr); Bastinec, J (Bastinec, Jaromir); Slavicek, T (Slavicek, Tomas); Hlustik, P (Hlustik, Petr); Brazdil, M (E Jiri)

Source: JOURNAL OF NEUROSCIENCE METHODS **Volume:** 318 **Pages:** 34-46 **DOI:** 10.1016/j.jneumeth.2019.02.012 **Published:**

Abstract: Background: Spatial and temporal resolution of brain network activity can be improved by combining different moda Resonance Imaging (fMRI) provides full brain coverage with limited temporal resolution, while electroencephalography (EEG), e high temporal resolution. Combining them may provide improved network characterization.
New Method: We examined relationships between EEG spatiospectral pattern timecourses and concurrent fMRI BOLD signals us response function (HRF) with 1st and 2nd temporal derivatives in voxel-wise general linear models (GLM). HRF shapes were deri courses during "resting-state", visual oddball and semantic decision paradigms.
Results: The resulting GLM F-maps self-organized into several different large-scale brain networks (LSBNs) often with different t revealed through differences in GLM-derived HRF shapes (e.g., with a lower time to peak than the canonical HRF). We demonstr spatiospectral patterns (related to concurrent fMRI) are weakly task-modulated.
Comparison with existing method(s): Previously, we demonstrated 14 independent EEG spatiospectral patterns within this EEG resting-state, visual oddball and semantic decision paradigms. Here, we demonstrate that their time courses are significantly co organized into LSBN structures. EEG-fMRI derived HRF peak appears earlier than the canonical HRF peak, which suggests limita canonical HRF shape in EEG-fMRI.
Conclusions: This is the first study examining EEG-fMRI relationships among independent EEG spatiospectral patterns over diffe highlight the importance of considering different HRF shapes when spatiotemporally characterizing brain networks using EEG a

Accession Number: WOS:000463294200004

PubMed ID: 30802472

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ISSN: 0165-0270

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Record 126 of 235

Title: Facile construction & modeling of a highly active thiacalixphenyl[4]arene-protected nano-palladium catalyst for various C
Author(s): Modi, K (Modi, Krunal); Patel, C (Patel, Chirag); Panchal, U (Panchal, Urvi); Liska, A (Liska, Alan); Kongor, A (Kongor, Ar VK (Jain, V. K.)
Source: NEW JOURNAL OF CHEMISTRY **Volume:** 43 **Issue:** 14 **Pages:** 5611-5622 **DOI:** 10.1039/c8nj05866k **Published:** APR 14 2(
Abstract: The design and creation of thiacalixphenyl[4]arene tetraacetohydrazide (TPTAH) has been utilized for the constructio (PdNps). The molecular modelling studies give an insight into the surface properties of TPTAH capped PdNps. The plausible red Pd(0) is due to the presence of hydrazide group on the periphery. The charge transfer for this reduction was initiated by the carb TPTAH behaves as a reducing and stabilizing agent for the formation of catalytically active TPTAH-PdNps that were characterize selected area electron diffraction (SAED), transmission electron microscopy (TEM), and powder X-ray diffraction. The TPTAH-Pd found to be catalytically active for C-C cross-coupling reactions such as the Suzuki-Miyaura, Heck, and Stille reactions. TPTAH-P conventional Pd catalyst in terms of yield, catalyst loading, reaction time, and recyclability.
Accession Number: WOS:000464280500037
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Patel, Chirag		0000-0003-0777-7720
Modi, Krunal	G-1015-2016	0000-0002-1151-1207
Liska, Alan	O-4810-2014	0000-0001-7107-6094

ISSN: 1144-0546
eISSN: 1369-9261

Record 127 of 235
Title: Remarkable variation of ribosomal DNA organization and copy number in gnetophytes, a distinct lineage of gymnosperm
Author(s): Wang, WC (Wang, Wencai); Wan, T (Wan, Tao); Becher, H (Becher, Hannes); Kuderova, A (Kuderova, Alena); Leitch, IJ ((Garcia, Sonia); Leitch, AR (Leitch, Andrew R.); Kovarik, A (Kovarik, Ales)
Source: ANNALS OF BOTANY **Volume:** 123 **Issue:** 5 **Pages:** 767-781 **DOI:** 10.1093/aob/mcy172 **Published:** APR 11 2019
Abstract: Introduction Gnetophytes, comprising the genera Ephedra, Gnetum and Welwitschia, are an understudied, enigmatic a controversial phylogenetic relationship to other seed plants. Here we examined the organization of ribosomal DNA (rDNA) acr Methods We applied high-throughput sequencing approaches to isolate and reconstruct rDNA units and to determine their intra addition, fluorescent in situ hybridization and Southern blot hybridization techniques were used to reveal the chromosome anc rDNA.
Key results The 5S and 35S rRNA genes were separate (S-type) in Gnetum montanum, Gnetum gnemon and Welwitschia mirabil Ephedra altissima. There was considerable variability in 5S rDNA abundance, ranging from as few as -4000 (W mirabilis) to >100 similar large variation was also observed in 5S rDNA locus numbers (two to 16 sites per diploid cell). 5S rRNA pseudogenes were functional genes forming a single unit in E. altissima and G. niontanum. Their copy number was comparable or even higher thar genes. In E. altissima internal transcribed spacers of 35S rDNA were long and intrinsically repetitive while in G. montanum and \ without the subrepeats.
Conclusions Gnetophytes are distinct from other gymnosperms and angiosperms as they display surprisingly large variability ir copy and locus numbers between genera, with no relationship between copy numbers and genome sizes apparent. Concerted e seems to have led to the amplification of 5S pseudogenes in both G. montanum and E. altissima. Evolutionary patterns of rDNA angiosperm features underlining the diversity of the group.
Accession Number: WOS:000483016800004
PubMed ID: 30265284
ISSN: 0305-7364
eISSN: 1095-8290

Record 128 of 235
Title: Chiral Surface from Achiral Ingredients: Modification of Cu(110) with Phthalic Acid
Author(s): Karageorgaki, C (Karageorgaki, Chrysanthi); Mutombo, P (Mutombo, Pingo); Jelinek, P (Jelinek, Pavel); Ernst, KH (Err
Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 123 **Issue:** 14 **Pages:** 9121-9127 **DOI:** 10.1021/acs.jpcc.9b00637 **Publis**
Abstract: The adsorption of dicarboxylic acids is a classical model approach for understanding molecular recognition at surface phthalic acid with an achiral Cu(110) surface has been investigated in ultrahigh vacuum by means of scanning tunneling micros diffraction, X-ray photoelectron spectroscopy, reflection absorption infrared spectroscopy, temperature-programmed desorptic theory. Different ordered domains at a length scale of several tens of nanometers are observed, of which three are enantiomorp two mirror-symmetric forms. Theoretical considerations suggest that spontaneous mirror-symmetry breaking occurs at the sing the surface becomes also chirally distorted.

Accession Number: WOS:000464768600071
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Mutombo, Pingo	G-5266-2014	0000-0002-8175-7587
Jelinek, Pavel	G-1542-2010	0000-0002-5645-8542

ISSN: 1932-7447

Record 129 of 235
Title: H-1 NMR is not a proof of hydrogen bonds in transition metal complexes
Author(s): Vicha, J (Vicha, J.); Foroutan-Nejad, C (Foroutan-Nejad, C.); Straka, M (Straka, M.)
Source: NATURE COMMUNICATIONS **Volume:** 10 **Article Number:** 1643 **DOI:** 10.1038/s41467-019-09625-9 **Published:** APR 9 20
Accession Number: WOS:000463872400019
PubMed ID: 30967536
Author Identifiers:

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Foroutan-Nejad, Cina	I-7512-2013	0000-0003-0755-8173

ISSN: 2041-1723

Record 130 of 235
Title: Rearrangement of meta-Bridged Calix[4]arenes Promoted by Internal Strain
Author(s): Slavik, P (Slavik, Petr); Krupicka, M (Krupicka, Martin); Eigner, V (Eigner, Vaclav); Vrzal, L (Vrzal, Lukas); Dvorakova, H (
(Lhotak, Pavel)
Source: JOURNAL OF ORGANIC CHEMISTRY **Volume:** 84 **Issue:** 7 **Pages:** 4229-4235 **DOI:** 10.1021/acs.joc.9b00107 **Published:** A
Abstract: The meta-bridged calixarenes possess a rigidified and highly distorted cavity, where the additional single-bond bridge strain on the whole system. As a consequence, these compounds exhibit a reasonably amended reactivity, compared with com which is governed by the release of internal strain. This can be documented by the reaction of the bridged calix[4]arene with P2 (apart from polymers) to a macrocyclic product with a rearranged basic skeleton. The methylene bridge next to the fluorene mo shifted from position 2 to position 4 of the phenolic subunit to minimize the tension. As revealed by single-crystal X-ray analysis residual dipolar coupling method, the rearrangement occurs without altering the original conformation.
Accession Number: WOS:000464250800046
PubMed ID: 30868881
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Eigner, Vaclav	G-5812-2014	0000-0003-1014-3980
Slavik, Petr	A-1100-2016	0000-0002-3326-6169

ISSN: 0022-3263

Record 131 of 235
Title: Pseudogap in the c-axis (along the ladder) optical conductivity of t - J ladders and its quasiparticle interpretation
Author(s): Karlubikova, P (Karlubikova, Paulina); Ruzickova, H (Ruzickova, Hana); Chaloupka, J (Chaloupka, Jiri); Munzar, D (Mu
Source: JOURNAL OF PHYSICS-CONDENSED MATTER **Volume:** 31 **Issue:** 13 **Article Number:** 135502 **DOI:** 10.1088/1361-648X/a
Abstract: Motivated by similarities between cuprate superconductors and two-leg ladder copper-oxide compounds and in orde understanding of optical properties of cuprate superconductors we have studied the c-axis (along the ladder) optical conductiv t(parallel to) - t(perpendicular to) - J(parallel to) - J(perpendicular to) two-leg ladder. Using exact diagonalization, we have calcu related quantities for cyclic ladders of up to 13 rungs. In agreement with results of an early study by Hayward and coworkers (H 53 8863) we find that sigma(omega) consists of a Drude peak at zero frequency and an absorption band in the infrared region th former by a pseudogap. The width of the pseudogap E-pG increases with increasing J/t, in parallel with an increase of the magr quasiparticle excitation spectra. Our central finding is that E-PG approximate to E-QP + Delta(s), where Delta(s) is the magnitud excitation spectra. We demonstrate that this approximate relation can be understood in terms of a phenomenological model in ladder and a coupling between charged quasiparticles and spin excitations. The relation is remarkably similar to the one betwe

energy scale of a dip in the in-plane optical conductivity, the superconducting gap 2 Delta and the energy of the spin-resonance (for a recent discussion of the optical data, see Sopik et al 2015 New J. Phys. 17 053022). Our findings support the point of view active excited states of cuprate superconductors can be viewed as consisting of two charged quasiparticles connected with pair excitation.

Accession Number: WOS:000458050100001

PubMed ID: 30625439

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Chaloupka, Jiri	I-3636-2014	
Chaloupka, Jiri		0000-0001-8898-0442

ISSN: 0953-8984

eISSN: 1361-648X

Record 132 of 235

Title: Exploiting sports-betting market using machine learning

Author(s): Hubacek, O (Hubacek, Ondrej); Sourek, G (Sourek, Gustav); Zelezny, F (Zelezny, Filip)

Source: INTERNATIONAL JOURNAL OF FORECASTING **Volume:** 35 **Issue:** 2 **Pages:** 783-796 **DOI:** 10.1016/j.ijforecast.2019.01.00

Abstract: We introduce a forecasting system designed to profit from sports-betting market using machine learning. We contribu ingredients. First, previous attempts to learn models for match-outcome prediction maximized the model's predictive accuracy these approaches, we also reduce the model's correlation with the bookmaker's predictions available through the published oc optimized model allows for better profit generation, and the approach is thus a way to 'exploit' the bookmaker. The second nov convolutional neural networks for match outcome prediction. The convolution layer enables to leverage a vast number of playe input. Thirdly, we adopt elements of the modern portfolio theory to design a strategy for bet distribution according to the odds trading off profit expectation and variance optimally. These three ingredients combine towards a betting method yielding posit experiments with NBA data from seasons 2007-2014 systematically, as opposed to alternative methods tested. (C) 2019 Internat Published by Elsevier B.V. All rights reserved.

Accession Number: WOS:000469310100030

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Hubacek, Ondrej		0000-0003-4449-0083

ISSN: 0169-2070

eISSN: 1872-8200

Record 133 of 235

Title: The plant Pontin and Reptin homologues, RuvBL1 and RuvBL2a, colocalize with TERT and TRB proteins in vivo, and partic biogenesis

Author(s): Schorova, S (Schorova, Sarka); Fajkus, J (Fajkus, Jiri); Zaveska Drabkova, L (Zaveska Drabkova, Lenka); Honys, D (Hor (Schrumpfova, Petra Prochazkova)

Source: PLANT JOURNAL **Volume:** 98 **Issue:** 2 **Pages:** 195-212 **DOI:** 10.1111/tpj.14306 **Published:** APR 2019

Abstract: Telomerase maturation and recruitment to telomeres is regulated by several telomerase- and telomere-associated pr proteins, human Pontin and Reptin play critical roles in telomerase biogenesis. Here we characterized plant orthologues of Pon RuvBL2a, respectively, and show association of Arabidopsis thaliana RuvBL1 (AtRuvBL1) with the catalytic subunit of telomeras vivo. In contrast to mammals, interactions between AtTERT and AtRuvBL proteins in A. thaliana are not direct and they are rath Arabidopsis thaliana Telomere Repeat Binding (AtTRB) proteins. We further show that plant orthologue of dyskerin, named AtC with AtTRB proteins but not with the AtRuvBL proteins in the plant nucleus/nucleolus, and interacts with the Protection of telor nucleolus or cytoplasmic foci. Our genome-wide phylogenetic analyses identify orthologues in RuvBL protein family within the of AtRuvBL genes in heterozygous T-DNA insertion A. thaliana mutants results in reduced telomerase activity and indicate the ir plant telomerase biogenesis.

Accession Number: WOS:000466782800002

PubMed ID: 30834599

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Drabkova, Lenka Zaveska	X-5699-2019	0000-0003-1140-6607
Fajkus, Jiri	D-2499-2012	0000-0002-3112-1716
Schorova, Sarka		0000-0003-2942-7051

ISSN: 0960-7412

eISSN: 1365-313X

Record 134 of 235

Title: Genetic and morphological variation in the circumpolar distribution range of Sphagnum warnstorfii: indications of vicaria peatmoss

Author(s): Yousefi, N (Yousefi, Narjes); Mikulaskova, E (Mikulaskova, Eva); Stenoien, HK (Stenoien, Hans K.); Flatberg, KI (Flatber (Kosuthova, Alica); Hajek, M (Hajek, Michal); Hassel, K (Hassel, Kristian)

Source: BOTANICAL JOURNAL OF THE LINNEAN SOCIETY **Volume:** 189 **Issue:** 4 **Pages:** 408-423 **DOI:** 10.1093/botlinnean/boy08

Abstract: The Quaternary climatic oscillations caused pronounced changes in the distribution of the genetic variation among p phenotypic diversification worldwide. However, how important these processes have been in plants with high gene flow potent Sphagnum warnstorfii is a peatmoss species with a wide circumpolar distribution range exhibiting considerable morphological Arctic plants differ morphologically from plants in the rest of its distribution range. We used single nucleotide polymorphism (S the patterns of genetic diversity in 112 plants from 105 localities sampled throughout the species distribution range and explor with phenotypic variation. Genetic cluster analysis identified two main genetic lineages with an average F-ST of 0.21 between th restricted to the Arctic region, whereas the second has a wider distribution range covering the Arctic, boreal and boreo-nemoral America. We show that morphological variation is mostly concordant with patterns of genetic differentiation, and possibly repr environments. Based on approximate Bayesian computation simulations, we find that the two lineages probably diverged from Glacial Maximum (LGM). Our results show that vicariance due to glacial oscillations probably played a role for current patterns o peatmoss exhibiting a high gene flow potential.

Accession Number: WOS:000464933400005

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Mikulaskova, Eva	AAE-3798-2019	0000-0002-6122-4265
Hajek, Michal	H-1648-2014	0000-0002-5201-2682

ISSN: 0024-4074

eISSN: 1095-8339

Record 135 of 235

Title: Non-adiabatic dynamics combining Ehrenfest, decoherence, and multiscale approaches applied to ionic rare-gas clusters ionization fragmentation, and collisions

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

Source: COMPUTATIONAL AND THEORETICAL CHEMISTRY **Volume:** 1153 **Pages:** 54-64 **DOI:** 10.1016/j.comptc.2019.02.016 **Pub**

Abstract: Methodological approaches for realistic modeling of non-adiabatic processes are reviewed and selected applications are based on a hybrid approach with heavy atomic nuclei treated classically and light electrons described quantum mechanica methodology consists in Ehrenfest's mean-field approach enhanced by a model inclusion of quantum decoherence. Approxima evolutions is also proposed for the cases where direct dynamical calculations become computationally impracticable. Specific of rare gases, based on effective, low-dimensional Hamiltonians built within the diatomics-in-molecules methodology, prove th of the developed methods in various fields like photodissociation, post-ionization fragmentation, and collisions.

Accession Number: WOS:000465058800007

ISSN: 2210-271X

eISSN: 1872-7999

Record 136 of 235

Title: Can All-Atom Molecular Dynamics Simulations Quantitatively Describe Homeodomain-DNA Binding Equilibria?

Author(s): Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 15 **Issue:** 4 **Pages:** 2635-2648 **DOI:** 10.1021/acs.jctc.8b0

Abstract: We systematically investigate the applicability of a molecular dynamics-based setup for the calculations of standard b biologically relevant protein-DNA complexes. The free energies are extracted from a potential of mean force calculated using ur Two protein-DNA systems derived from a homeodomain transcription factor complex are studied in order to investigate the bin globular proteins. Free energies and trajectories obtained using two modern molecular mechanical force fields are compared to experimental data. The temperature dependence of the calculated standard binding free energies is investigated by performing of temperatures. We show that the values of standard binding free energies obtained from these simulations are overestimated results. Significant differences are observed between the two protein-DNA systems and between the two force fields, which are propensities to form inter- and intramolecular contacts. The number of protein-DNA contacts increases with increasing tempera experimentally known temperature dependence of enthalpies of binding. However, conclusions about the temperature depend free energies cannot be made with confidence, as the differences among the values are on the order of statistical uncertainty.

Accession Number: WOS:000464475500043

PubMed ID: 30807142

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

ISSN: 1549-9618

eISSN: 1549-9626

Record 137 of 235

Title: Divergence between bread wheat and Triticum militinae in the powdery mildew resistance QPm.tut-4A locus and its impli resistance gene

Author(s): Janakova, E (Janakova, Eva); Jakobson, I (Jakobson, Irena); Peusha, H (Peusha, Hilma); Abrouk, M (Abrouk, Michael); Monika); Simkova, H (Simkova, Hana); Safar, J (Safar, Jan); Vrana, J (Vrana, Jan); Dolezel, J (Dolezel, Jaroslav); Jarve, K (Jaerve, Miroslav)

Source: THEORETICAL AND APPLIED GENETICS **Volume:** 132 **Issue:** 4 **Pages:** 1061-1072 **DOI:** 10.1007/s00122-018-3259-3 **Publ**

Abstract: A segment of Triticum militinae chromosome 7G harbors a gene(s) conferring powdery mildew resistance which is eff and the adult plant stages when transferred into bread wheat (T. aestivum). The introgressed segment replaces a piece of whea analysis of segregating materials generated to positionally clone the gene highlighted that in a plant heterozygous for the introg limited recombination occurs between the introgressed region and bread wheat 4A. Nevertheless, 75 genetic markers were suc region, thereby confining the gene to a 0.012cM window along the 4AL arm. In a background lacking the Ph1 locus, the localized raised 33-fold, enabling the reduction in the length of the region containing the resistance gene to a 480 kbp stretch harboring substituted segment in the reference sequence of bread wheat cv. Chinese Spring is longer (640 kbp) and harbors 16 genes. A co sequences revealed a high degree of divergence with respect to both their gene content and nucleotide sequence. Of the 12 T. n a homolog in cv. Chinese Spring. Possible candidate genes for the resistance have been identified based on function predicted f

Accession Number: WOS:000463674000016

PubMed ID: 30535646

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Jarve, Kadri		0000-0002-4970-8689
Abrouk, Michael	F-8516-2014	0000-0001-9082-1432

ISSN: 0040-5752

eISSN: 1432-2242

Record 138 of 235

Title: Modelling of cracking of the ceramic foam specimen with a central notch under the tensile load

Author(s): Sevecek, O (Sevecek, Oldrich); Bertolla, L (Bertolla, Luca); Chlup, Z (Chlup, Zdenek); Rehorek, L (Rehorek, Lukas); Ma Marcian, P (Marcian, Petr); Kotoul, M (Kotoul, Michal)

Source: THEORETICAL AND APPLIED FRACTURE MECHANICS **Volume:** 100 **Pages:** 242-250 **DOI:** 10.1016/j.tafmec.2019.01.024 **F**

Abstract: In this contribution, open cell ceramic foam structures composed of regular/irregular shape cells and containing a ma were investigated in terms of their cracking upon the tensile loading and their strength was predicted using the FE simulations. real ceramic foam specimen containing a central notch/crack was subjected to a tension, resulting in a failure beginning at the t

discusses an approach how to predict the critical failure load and also the crack path in the foam structure. Various cell irregula macroscopic notch was considered in the investigations. Predictions of the foam structure cracking were performed using the b having characteristics of the real foam structure and by utilization of the stress criterion which considers failure of particular str stress on them reaches the tensile strength of the ceramic material. Outputs from simulations were compared with available ex with an estimation of the critical failure load calculated using the developed analytical model.

Accession Number: WOS:000462107700025

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rehorek, Lukas	P-8243-2019	0000-0002-7026-7216
Marcian, Petr	E-7359-2017	0000-0002-9458-9690
Chlup, Zdenek	H-5290-2011	0000-0002-6117-240X

ISSN: 0167-8442

eISSN: 1872-7638

Record 139 of 235

Title: LDA plus U Calculation of Electronic and Thermoelectric Properties of Doped Tetrahedrite Cu12Sb4S13

Author(s): Knizek, K (Knizek, K.); Levinsky, P (Levinsky, P.); Hejtmanek, J (Hejtmanek, J.)

Source: JOURNAL OF ELECTRONIC MATERIALS **Volume:** 48 **Issue:** 4 **Pages:** 2018-2021 **DOI:** 10.1007/s11664-019-06960-x **Publi**

Abstract: Tetrahedrite-based thermoelectric materials have received much attention in recent years due to their good thermoel earth-abundance. The parent compound Cu12Sb4S13 exhibits a high power factor and low lattice thermal conductivity. Further thermoelectric figure of merit ZT is expected in substituted compounds, primarily at the Cu site Cu12-xMxSb4S13. In this work v substitution effects on thermoelectric properties using density-functional theory electronic structure calculations in combinati electrical transport properties by the BoltzTrap program.

Accession Number: WOS:000460453100032

Conference Title: 37th International Conference on Thermoelectrics (ICT)

Conference Date: JUL 01-05, 2018

Conference Location: Caen, FRANCE

ISSN: 0361-5235

eISSN: 1543-186X

Record 140 of 235

Title: Phylogenomics of pike cichlids (Cichlidae: Crenicichla) of the C. mandelburgeri species complex: rapid ecological speciati high endemism in the Middle Parana basin

Author(s): Pialek, L (Pialek, Lubomir); Burress, E (Burress, Edward); Dragova, K (Dragova, Klara); Almiron, A (Almiron, Adriana); C Rican, O (Rican, Oldrich)

Source: HYDROBIOLOGIA **Volume:** 832 **Issue:** 1 **Special Issue:** SI **Pages:** 355-375 **DOI:** 10.1007/s10750-018-3733-6 **Published:**

Abstract: The Crenicichla mandelburgeri species complex from the Middle Parana basin is a diverse group of cichlid species and ecomorphs found within the entire genus Crenicichla. Here, we study the phylogenetic relationships within the C. mandelburge ddRAD sequencing with focus on its two candidate species flocks endemic to the Iguazu and Urugua-i Rivers, and on two putati Piray Guazu River. These species flocks include four and three syntopic species, respectively, which are strongly adapted to diffe include derived ecomorphs of Crenicichla (molluscivores, a periphyton grazer, and a crevice-feeding thick-lipped invertivore). C strongly support monophyly and rapid diversification of the Iguazu species flock, but reveal more complex evolutionary histori Guazu tributaries. Most species in the Middle Parana, including one species in the Urugua-i and both species in the Piray Guazu discordance, and in both of these tributaries, we also found hybridization in one of the resident species. Population-level analys of the Iguazu species and coupled with their dramatic ecological diversity, this radiation exemplifies characteristics of a species ecological speciation.

Accession Number: WOS:000459429800020

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pialek, Lubomir	G-4611-2015	0000-0003-1881-4646
Rican, Oldrich		0000-0001-9513-0446

ISSN: 0018-8158

eISSN: 1573-5117

Record 141 of 235

Title: A new pelagic predatory pike cichlid (Teleostei: Cichlidae: Crenicichla) from the C. mandelburgeri species complex with pa evolution

Author(s): Pialek, L (Pialek, Lubomir); Casciotta, J (Casciotta, Jorge); Almiron, A (Almiron, Adriana); Rican, O (Rican, Oldrich)

Source: HYDROBIOLOGIA **Volume:** 832 **Issue:** 1 **Special Issue:** SI **Pages:** 377-395 **DOI:** 10.1007/s10750-018-3754-1 **Published:**

Abstract: The Crenicichla mandelburgeri species complex from the Middle Parana shows parallel evolution of ecomorphs to the species complex from the Uruguay River. In this article, we describe a new species from the C. mandelburgeri species complex t morphology and ecology to an unrelated species from the C. missioneira species complex (C. celidochilus). The new species is a predominantly on fishes and together with C. celidochilus is the only known pelagic species in the large riverine genus Crenicicl endemic solely to a small tributary (the Urugua-i) of the Middle Parana River where it is sympatric and partly syntopic with two species that, however, differ strongly in their ecomorphologies (one is a generalistic invertivore and the other a specialized mol phylogeny finds the new species nested within the widespread C. mandelburgeri. Reduced genome-representation ddRAD anal that this new species is of a hybrid origin and shares ancestry with C. ypo, one of the two studied sympatric species.

Accession Number: WOS:000459429800021

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Pialek, Lubomir	G-4611-2015	0000-0003-1881-4646
Rican, Oldrich		0000-0001-9513-0446

ISSN: 0018-8158

eISSN: 1573-5117

Record 142 of 235

Title: High nonassociativity in order 8 and an associative index estimate

Author(s): Drapal, A (Drapal, Ales); Valent, V (Valent, Viliam)

Source: JOURNAL OF COMBINATORIAL DESIGNS **Volume:** 27 **Issue:** 4 **Pages:** 205-228 **DOI:** 10.1002/jcd.21632 **Published:** APR 2

Abstract: Let Q be a quasigroup. Put a(Q) = vertical bar{(x, y, z) is an element of Q(3); x(yz)) = (xy)z}vertical bar and assume that v Let delta(L) and delta(R) be the number of left and right translations of Q that are fixed point free. Put delta(Q) = delta(L) + delta number of idempotents of Q. It is shown that a(Q) >= 2n - i(Q) + delta(Q). Call Q extremely nonassociative if a(Q) = 2n - i(Q). The p be the first known example of such a quasigroup, with n = 8, a(Q) = 16, and i(Q) = 0. It also provides supporting theory for a searc all quasigroups of order 8.

Accession Number: WOS:000459631700001

ISSN: 1063-8539

eISSN: 1520-6610

Record 143 of 235

Title: Magnetism of 4f-atoms adsorbed on metal and graphene substrates

Author(s): Shick, AB (Shick, A. B.); Denisov, AY (Denisov, A. Yu.)

Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 475 **Pages:** 211-215 **DOI:** 10.1016/j.jmmm.2018.11.078

Abstract: The electronic structure and magnetism of individual Dy atom adsorbed on the graphene/Ir(1 1 1) surface is investigat the density functional theory with the Hubbard-I approximation to the Anderson impurity model (DFT + HIA). The divalent Dy2+ magnetic moment of 9.4-9.6 mu(B), depending on the placement of the graphene on the Ir(1 1 1) surface, in an external magnet magnetic moments are evaluated, and compared with the X-ray magnetic circular dichroism (XMCD) data. The positive magneti determines the out-of-plane orientation of the Dy adatom magnetic moment. Without an external magnetic field, the ground st = 8, J(z) = +/- 7.9 >, symmetry protected from quantum tunnelling of the magnetization. Calculations show that insertion of the reduction of the hybridization between Dy-4f-states and the Ir(1 1 1) substrate, and leads to increase of the magnetic moment r adatom.

Accession Number: WOS:000458152000034

Conference Title: 9th Joint European Magnetic Symposia (JEMS)

Conference Date: SEP 03-07, 2018

Conference Location: Mainz, GERMANY

Author Identifiers:

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Shick, Alexander	C-1420-2013	0000-0003-2700-5517

ISSN: 0304-8853

eISSN: 1873-4766

Record 144 of 235

Title: Alloy disorder and fluctuating magnetic moments in the Earth's core

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

Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 475 **Pages:** 767-771 **DOI:** 10.1016/j.jmmm.2018.11.112

Abstract: The electronic and thermal transport properties of the Earth's core are crucial for many geophysical models such as t
Earth's magnetic field. We show by first-principles modeling and methods of statistical physics that the spin disorder, not consi
gives an essential contribution to the electrical resistivity at the Earth's core conditions. The origin of this spin-disorder resistivi
existence of fluctuating local moments that are stabilized at high temperatures by the magnetic entropy even at pressures at wl
non-magnetic. It turns out that the contributions of various scattering mechanisms (alloy disorder, phonon scattering, spin disc
correlations) are comparable, but not additive. Here we report results for iron and iron-rich alloys (Fe-O, Fe-Si, Fe-S) that can be
Special attention is paid to alloys with two magnetic elements (Fe-Ni).

Accession Number: WOS:000458152000109

Conference Title: 9th Joint European Magnetic Symposia (JEMS)

Conference Date: SEP 03-07, 2018

Conference Location: Mainz, GERMANY

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Turek, Ilja	G-5553-2014	0000-0002-0604-6590
KUDRNOVSKY, Josef	G-5581-2014	0000-0002-9968-6748

ISSN: 0304-8853

eISSN: 1873-4766

Record 145 of 235

Title: Chronic exposure of bumblebees to neonicotinoid imidacloprid suppresses the entire mevalonate pathway and fatty acid

Author(s): Erban, T (Erban, Tomas); Sopko, B (Sopko, Bruno); Talacko, P (Talacko, Pavel); Harant, K (Harant, Karel); Kadlikova, K
T (Halesova, Tatana); Riddellova, K (Riddellova, Katerina); Pekas, A (Pekas, Apostolos)

Source: JOURNAL OF PROTEOMICS **Volume:** 196 **Pages:** 69-80 **DOI:** 10.1016/j.jprot.2018.12.022 **Published:** MAR 30 2019

Abstract: Determining the side effects of pesticides on pollinators is an important topic due to the increasing loss of pollinators
effects of chronic sublethal exposure of the neonicotinoid pesticide imidacloprid on the bumblebee Bombus terrestris under la
analytical standard of imidacloprid in sugar solution was used for the treatment. Verification of pesticides using UHPLC-QqQ-M
bumblebees showed the presence of only two compounds, imidacloprid and imidacloprid-olefin, which were found in quantiti
0.43 ng/g, respectively. Thus, the level of the dangerous metabolite imidacloprid-olefin was 3.4-fold higher than that of imidacl
MS/MS quantitative proteomics of bumblebee heads enabled quantitative comparison of 2883 proteins, and 206 proteins were
imidacloprid treatment. The next analysis revealed that the highly downregulated markers are members of the terpenoid backb
(KEGG: bter00900) and that imidacloprid treatment suppressed the entire mevalonate pathway, fatty acid synthesis and associa
results indicate that the consequences of imidacloprid treatment are complex, and the marker changes are associated with me
diseases and olfaction disruption. This study provides important markers and can help to explain the widely held assumptions
Significance: The major finding is that all markers of the mevalonate pathway were substantially downregulated due to the chro
The disbalance of mevalonate pathway has many important consequences. We suggest the mechanism associated with the nov
imidacloprid. The results are helpful to explain that imidacloprid impairs the cognitive functions and possesses the delayed an

Accession Number: WOS:000460716800007

PubMed ID: 30583045

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sopko, Bruno	N-7345-2018	0000-0002-5580-1871
Erban, Tomas	F-9615-2011	0000-0003-1730-779X
Harant, Karel	L-2052-2014	0000-0002-9654-5392

ISSN: 1874-3919

eISSN: 1876-7737

Record 146 of 235

Title: Collinearly improved kernel suppresses Coulomb tails in the impact-parameter dependent Balitsky-Kovchegov evolution

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

Source: PHYSICAL REVIEW D **Volume:** 99 **Issue:** 5 **Article Number:** 051502 **DOI:** 10.1103/PhysRevD.99.051502 **Published:** MAR

Abstract: We solved the impact-parameter dependent Balitsky-Kovchegov equation with the recently proposed collinearly impr solutions do not present the Coulomb tails that have affected previous studies. We also show that once choosing an adequate i to obtain a reasonable description of HERA data on the structure function of the proton, as well as on the cross section for the e vector meson off proton targets. As a further application of the solutions, we computed the impact-parameter dependent Weizs distribution.

Accession Number: WOS:000462915500001

ISSN: 2470-0010

eISSN: 2470-0029

Record 147 of 235

Title: Collective Modes in Excitonic Magnets: Dynamical Mean-Field Study

Author(s): Geffroy, D (Geffroy, D.); Kaufmann, J (Kaufmann, J.); Hariki, A (Hariki, A.); Gunacker, P (Gunacker, P.); Hausoel, A (Hau

Source: PHYSICAL REVIEW LETTERS **Volume:** 122 **Issue:** 12 **Article Number:** 127601 **DOI:** 10.1103/PhysRevLett.122.127601 **Pu**

Abstract: We present a dynamical mean-field study of dynamical susceptibilities in the two-band Hubbard model. Varying the r the two-particle excitations in the normal as well as in the ordered phase, an excitonic condensate. The two-particle dynamical the ordered phase reveal the gapless Goldstone modes arising from spontaneous breaking of continuous symmetries. We also c mode, characterized by vanishing of the gap at the phase boundary. Qualitative changes observed in the spin susceptibility can probe to identify the excitonic condensation.

Accession Number: WOS:000462936100014

PubMed ID: 30978073

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Gunacker, Patrik		0000-0002-7593-2529

ISSN: 0031-9007

eISSN: 1079-7114

Record 148 of 235

Title: Influence of 3D Spruce Tree Representation on Accuracy of Airborne and Satellite Forest Reflectance Simulated in DART

Author(s): Janoutova, R (Janoutova, Ruzena); Homolova, L (Homolova, Lucie); Malenovsky, Z (Malenovsky, Zbynek); Hanus, J (H Nicolas); Gastellu-Etchegorry, JP (Gastellu-Etchegorry, Jean-Philippe)

Source: FORESTS **Volume:** 10 **Issue:** 3 **Article Number:** 292 **DOI:** 10.3390/f10030292 **Published:** MAR 26 2019

Abstract: Advances in high-performance computer resources and exploitation of high-density terrestrial laser scanning (TLS) da close-to-reality 3D forest scenes for use in canopy radiative transfer models. Consequently, our main objectives were (i) to recor Norway spruce (Picea abies) trees by deriving distribution of woody and foliage elements from TLS and field structure data and 3D spruce representations for evaluation of the effects of canopy structure on forest reflectance simulated in the Discrete Anisot (DART) model. Data for this study were combined from two spruce research sites located in the mountainous areas of the Czech structure effects on simulated top-of-canopy reflectance were evaluated for four scenarios (10 x 10 m scenes with 10 trees), rang simple to highly detailed architectures. First scenario A used predefined simple tree crown shapes filled with a turbid medium v branches. Other three scenarios used the reconstructed 3D spruce representations with B detailed needle shoots transformed i simplified shoots retained as facets, and D with detailed needle shoots retained as facets D. For the first time, we demonstrated model to simulate reflectance of complex coniferous forest scenes up to the level of a single needle (scenario D). Simulated bidi extracted for each scenario were compared with actual airborne hyperspectral and space-borne Sentinel-2 MSI reflectance data largest differences from the remote sensing observations, mainly in the visible and NIR regions, whereas scenarios B, C, and D p revealing a good agreement with the remote sensing data. When judging the computational requirements for reflectance simul be considered as most operational spruce forest representation, because the transformation of 3D shoots in turbid medium red simulation time and hardware requirements.

Accession Number: WOS:000464462400002
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Malenovsky, Zbynek	A-7819-2011	0000-0002-1271-8103
Janoutova, Ruzena	G-2755-2014	0000-0003-1830-7556
Homolova, Lucie	A-8436-2011	0000-0001-7455-2834

ISSN: 1999-4907

Record 149 of 235
Title: Surface of aqueous solutions of alkali halides: layer by layer analysis
Author(s): Skvara, J (Skvara, Jiri); Nezbeda, I (Nezbeda, Ivo)
Source: MOLECULAR SIMULATION **Volume:** 45 **Issue:** 4-5 **Special Issue:** SI **Pages:** 358-372 **Article Number:** UNSP 144705 **DOI:** 10.1080/08927022.2018.1540871 **Published:** MAR 24 2019
Abstract: Interfacial layers of both vapour/liquid and crystal/liquid aqueous solutions of sodium and caesium halides have bee different methods for the identification of interfacial molecules and layers, and both non-polarisable and polarisable models. It methods yields a somewhat different result with the best mutual agreement found between the ITIM (Identification of Truly Int shape-based USTI (Universal Scheme for Triangulated Interfaces) methods. Concerning the water models, the commonly used Cheatham, J. Phys. Chem. 112 (2008) 9020] model predicts the structural properties of the vapor/liquid interface different from MADRID and polarisable AH/BK3 models, and also from experiment. The same applies also to the structural properties of the sc the AH/BK3 and JC models yield a surplus of chlorine ions, a segregation of Na and Cl- ions in the interfacial layers predicted by in the polarisable model.
Accession Number: WOS:000460668700011
ISSN: 0892-7022
eISSN: 1029-0435

Record 150 of 235
Title: Tuning of the gold work function by carborane films studied using density functional theory
Author(s): Hladik, M (Hladik, Martin); Vetushka, A (Vetushka, Aliaksei); Fejfar, A (Fejfar, Antonin); Vazquez, H (Vazquez, Hector)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 21 **Issue:** 11 **Pages:** 6178-6185 **DOI:** 10.1039/c9cp00346k **Publishe**
Abstract: Using density functional theory including van der Waals interactions, we calculate the adsorption and electronic prop closo-dodecaboranes chemisorbed on Au(111) surfaces. Carborane molecules consist of a cage-like structure made of boron ar a large intrinsic dipole. We consider two functionalized carborane positional isomers, with thiol linker groups attached to eithe atoms, such that when adsorbed on the Au substrate, the molecular dipole points towards the metal surface or away from it. W of junction geometries and find that carborane adsorption can induce significant changes in the work function of the Au substra changes depend strongly on the interface geometry at the atomistic level. From the analysis of these junction structures, we pr mechanisms that determine adsorption geometries, and relate them to interface electronic structure and resulting work functi our results highlight the important role played in these interface quantities by distortions in the Au surface layer induced by car
Accession Number: WOS:000462659300030
PubMed ID: 30821802
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Fejfar, Antonin	A-3347-2009	0000-0003-0988-0772
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922

ISSN: 1463-9076
eISSN: 1463-9084

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Page 4 (Records 151 -- 200)
[1 | 2 | 3 | 4 | 5]

Record 151 of 235

Title: Synthesis and characterisation of palladium(ii) complexes with hybrid phosphinoferrocene ligands bearing additional O-d

Author(s): Vosahlo, P (Vosahlo, Petr); Schulz, J (Schulz, Jiri); Skoch, K (Skoch, Karel); Cisarova, I (Cisarova, Ivana); Stepnicka, P (

Source: NEW JOURNAL OF CHEMISTRY **Volume:** 43 **Issue:** 11 **Pages:** 4463-4470 **DOI:** 10.1039/c9nj00298g **Published:** MAR 21 2

Abstract: While 1,1'-bis(diphenylphosphino) ferrocene (dppf) is widely used as a ligand in coordination chemistry and catalysis containing functional groups have long been overlooked. Accordingly, we studied the coordination behaviour in Pd(II) complex phosphinoferrocene ligands bearing secondary O-donor groups, Ph2PfcR, wherein R = CHO (1), Ac (2) and CMe2(OH) (3), and fc Depending on the stoichiometry, reactions of 1-3 (L) with [PdCl2(cod)] (cod = eta(2):eta(2)-cycloocta-1,5-diene) produced the re dipalladium complexes, trans[PdCl2(L-kappa P)(2)] and trans-[PdCl(mu-Cl)(L-kappa P)](2). Compound [PdCl(mu-Cl)(3-kappa P) readily, giving rise to [PdCl(mu-Cl)(Ph(2)PfcC(Me)=CH2-kappa P)](2). Furthermore, ligands 1-3 cleaved [(L-NC)Pd(mu-Cl)](2) (L-N N)methyl)phenyl-kappa C-1), yielding [(L-NC)PdCl(L-kappa P)], which were converted into the cationic complexes [(L-NC)PdCl(L 3/PF6). Compounds with ligands 1 and 2 were structurally authenticated as stable bis-chelate complexes. In contrast, the produ rather unstable and converted into [(L-NC)Pd(AcOEt-kappa O)(3-kP)][PF6] upon recrystallisation. Weak oxygen coordination wa [(L-NC)PdCl(L)] X with (PhCH2NEt3)Cl in which the parent chloride complexes were regenerated, and this was further corrobora findings, pointing to hemilabile coordination of 1-3, are relevant for catalysis because de-coordination of the weaker binding O- vacant site for a substrate, thereby enhancing the catalytic properties of metal complexes with ligands of this type.

Accession Number: WOS:000460972700016

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Vosahlo, Petr	U-4827-2017	0000-0003-0981-3676
Stepnicka, Petr	E-3465-2010	0000-0002-5966-0578

ISSN: 1144-0546

eISSN: 1369-9261

Record 152 of 235

Title: Calculations of the Lu3N@C-80 two-isomer equilibrium

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

Source: FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES **Volume:** 27 **Issue:** 5 **Pages:** 382-386 **DOI:** 10.1080/15363

Access Date: MAR 2019 **Published:** MAY 4 2019

Abstract: Computations of the relative concentrations are reported for the two isomers of Lu3N@C-80 experimentally known, i. into the isolated-pentagon-rule (IPR) C-80 cages with I-h and symmetries. The calculations are mostly based on the density-fun treatments with the B3LYP functional. The inter-isomeric energetics is further refined with the MP2 perturbation method which in the potential energy by 16.9 kcal/mol. The isomeric populations are evaluated using the Gibbs energy in a broad temperature performed with the floating-encapsulate-model (FEM) treatment can reasonably reproduce the observed isomeric ratio, thus p adequate representation of the dynamic endohedral symmetry.

Accession Number: WOS:000463533000001

ISSN: 1536-383X

eISSN: 1536-4046

Record 153 of 235

Title: Molecular Techniques Complement Culture-Based Assessment of Bacteria Composition in Mixed Biofilms of Urinary Tract

Author(s): Kotaskova, I (Kotaskova, Iva); Obrucova, H (Obrucova, Hana); Malisova, B (Malisova, Barbora); Videnska, P (Videnska, (Zwinsova, Barbora); Peroutkova, T (Peroutkova, Tereza); Dvorackova, M (Dvorackova, Milada); Kumstat, P (Kumstat, Petr); Troja (Ruzicka, Filip); Hola, V (Hola, Veronika); Freiberger, T (Freiberger, Tomas)

Source: FRONTIERS IN MICROBIOLOGY **Volume:** 10 **Article Number:** 462 **DOI:** 10.3389/fmicb.2019.00462 **Published:** MAR 20 2(

Abstract: Urinary or ureteral catheter insertion remains one of the most common urological procedures, yet is considered a pre tract infection. Diverse bacterial consortia adhere to foreign body surfaces and create various difficult to treat biofilm structures catheter- and stent-related samples, treated with sonication, using both routine culture and broad-range 16S rDNA PCR followe Electrophoresis and Sanger sequencing (PCR-DGGE-S). In 29 selected samples, 16S rRNA amplicon Illumina sequencing was per methods were compared. In 338 positive samples, from which 86.1% were polybacterial, 1,295 representatives of 153 unique O

positive microbes were found in 46.5 and 59.1% of catheter- and stent-related samples, respectively. PCR-DGGE-S was shown as higher overall specificity (95 vs. 85%, p < 0.01) though lower sensitivity (50 vs. 69%, p < 0.01) in comparison to standard culture. considerably widened a spectrum of microbes detected in biofilms, including the very prevalent emerging opportunistic patho Using massive parallel sequencing as a reference method in selected specimens, culture combined with PCR-DGGE was shown tool for determining the composition of urinary catheter-related biofilms. This might be applicable particularly to immunocom catheter-colonizing bacteria may lead to severe infectious complications. For the first time, broad-range molecular detection se evaluated in this setting. This study extends the knowledge of biofilm consortia composition by analyzing large urinary catheter both molecular and culture techniques, including the widest dataset of catheter-related samples characterized by 16S rRNA am

Accession Number: WOS:000461804900001

PubMed ID: 30949137

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kotaskova, Iva		0000-0002-6336-6742

ISSN: 1664-302X

Record 154 of 235

Title: Norcorrole as a Delocalized, Antiaromatic System

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

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 4852 **DOI:** 10.1038/s41598-019-39972-y **Published:** MAR 19 2019

Abstract: Nickel norcorrole provides an unusual example of a molecule that is strongly antiaromatic according to the magnetic according to high-quality DFT calculations, a symmetric, delocalized structure with no difference in bond length between adjac fragment molecular orbital analysis suggests that these discordant observations are a manifestation of the high stability of the retain their electronic and structural integrity even as part of the norcorrole ring system.

Accession Number: WOS:000461563200012

PubMed ID: 30890733

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Conradie, Jeanet	O-1838-2019	0000-0002-8120-6830
Ghosh, Abhik	G-8164-2016	0000-0003-1161-6364

ISSN: 2045-2322

Record 155 of 235

Title: Square-Planar Pt(II) and Ir(I) Complexes as the Lewis Bases: Donor-Acceptor Adducts with Group 13 Trihalides and Trihyd

Author(s): Chval, Z (Chval, Zdenek); Dvorackova, O (Dvorackova, Olga); Chvalova, D (Chvalova, Daniela); Burda, JV (Burda, Jaros

Source: INORGANIC CHEMISTRY **Volume:** 58 **Issue:** 6 **Pages:** 3616-3626 **DOI:** 10.1021/acs.inorgchem.8b02765 **Published:** MAR

Abstract: The stability and properties of donor acceptor adducts of square-planar Pt(II) and Ir(I) complexes (designated as PtX, complexes) with trihydrides and trihalides of group 13 elements of general formula YZ(3) (Y = B, Al, Ga; Z = H, F, Cl, Br) were stud methodology in the gas phase. MX complexes were represented by wide range of the ligand environment which included mode and cis-[Pt(NH3)(2)X-2](0) (X = H, CH3, F, Cl, Br) and isoelectronic complexes [Ir(NNN)(CH3)](0) and [Pt(NCN)(CH3)](0) with trider ligands. MX complexes acted as the Lewis bases donating electron density from the doubly occupied 5d(z)(2) M = Ira), Pt(II) Y = E metal M atom to the empty valence p, orbital of Y whose evidence was clearly provided by the natural atomic orbital (NAO) anal to the formation of pentacoordinated square pyramidal MX"(YZ3) adducts with M"Y dative bond. Binding energies were 44.7 an of GaF3 as the strongest acid with PtNCN and IrNNN pincer ligands complexes. Only M.13 bonds had covalent character althoug least stable due to large values of Pauli repulsion and deformation energies. The highest degree of covalent character was foun series of structures studied. Al and Ga adducts showed remarkably similar behavior with respect to geometry and binding ener

Accession Number: WOS:000461978700012

PubMed ID: 30816711

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Dvorackova, Olga	D-8967-2016	0000-0001-9980-6992
Chvalova, Daniela	R-3194-2018	

Chval, Zdenek	D-8964-2016	0000-0003-1922-8390
bUrda, Jaroslav	C-9199-2009	0000-0001-9909-8797

ISSN: 0020-1669

eISSN: 1520-510X

Record 156 of 235

Title: NMR and ab initio study of gallium metal under pressure

Author(s): Reznicek, R (Reznicek, R.); Chlan, V (Chlan, V); Haase, J (Haase, J.)

Source: PHYSICAL REVIEW B **Volume:** 99 **Issue:** 12 **Article Number:** 125121 **DOI:** 10.1103/PhysRevB.99.125121 **Published:** MAI

Abstract: Gallium metal possesses a complex phase diagram and it has been the subject of many experimental and theoretical hyperfine properties of its phases requiring higher pressure beyond the liquid-I-II triple point were seldom examined. In this wo liquid and solid gallium metal under pressure are investigated by nuclear magnetic resonance (NMR) measurements and ab init field gradient and NMR shift of the Ga-III phase are both measured and calculated and their relation to electronic structure is int calculations of pressure dependencies of the hyperfine parameters of several other solid gallium phases are presented.

Accession Number: WOS:000461962900002

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Chlan, Vojtech	D-4868-2017	0000-0001-6963-9273

ISSN: 2469-9950

eISSN: 2469-9969

Record 157 of 235

Title: Surface-induced magnetism in intermetallics: Ni3Ge compound as a case study

Author(s): Meng, FS (Meng, Fan-Shun); Vsianska, M (Vsianska, Monika); Friak, M (Friak, Martin); Sob, M (Sob, Mojmir)

Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 474 **Pages:** 273-281 **DOI:** 10.1016/j.jmmm.2018.11.055

Abstract: By means of the first-principles calculations we investigate the magnetic properties of four low-index surfaces in the b intermetallic compound with the L1(2) structure. We predict that the (1 1 1) surface of Ni3Ge is magnetically ordered, with all m the Ni sites. Magnetic order is also found at the Ni-terminated (0 01), (1 1 0) and (2 1 0) surfaces, however, the nonmagnetic NiGe more stable similarly as in other L1(2) compounds. It turns out that the magnetic order in the bulk Ni3Ge is destroyed complete and Ni-d states and it is recovered at some surfaces due to the reduced coordinate number of Ni atoms. We also report on a par magnetization at the Ni3Ge(1 1 1) surface where the ferromagnetic and anti-ferromagnetic-like states are degenerated because layers between the two magnetic surfaces and there is no interference between them. The calculated results obtained for Ni3Ge Ni3Al; the differences between these two compounds are discussed.

Accession Number: WOS:000459494600039

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Vsianska, Monika	O-7454-2015	
Sob, Mojmir	G-6865-2011	0000-0002-5724-890X

ISSN: 0304-8853

eISSN: 1873-4766

Record 158 of 235

Title: Tetragonal CuMnAs alloy: Role of defects

Author(s): Maca, F (Maca, F.); Kudrnovsky, J (Kudrnovsky, J.); Balaz, P (Balaz, P.); Drchal, V (Drchal, V.); Carva, K (Carva, K.); Turek

Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 474 **Pages:** 467-471 **DOI:** 10.1016/j.jmmm.2018.10.145

Abstract: The antiferromagnetic (AFM) CuMnAs alloy with tetragonal structure is a promising material for the AFM spintronics. T indicate the presence of defects. We confirmed vacancies on Mn or Cu sublattices and Mncu and Cum antisites as most probable new ab initio total energy calculations. We have estimated resistivities of possible defect types as well as resistivities of samples analysis is available. In the latter case we have found that samples with Cu- and Mn-vacancies with low formation energies have well with the experiment. Finally, we have also calculated exchange interactions and estimated the Neel temperatures by using good agreement with experiment was obtained.

Accession Number: WOS:000459494600068

Conference Title: 9th Joint European Magnetic Symposia (JEMS)

Conference Date: SEP 03-07, 2018
Conference Location: Mainz, GERMANY
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Maca, Frantisek	G-4467-2014	0000-0002-8004-9132
Carva, Karel	A-3703-2008	0000-0002-2275-1986
KUDRNOVSKY, Josef	G-5581-2014	0000-0002-9968-6748
Turek, Ilja	G-5553-2014	0000-0002-0604-6590
Balaz, Pavel	M-9510-2015	0000-0003-0016-9271

ISSN: 0304-8853
eISSN: 1873-4766

Record 159 of 235
Title: Electrical transport with temperature-induced spin disorder in NiMnSb
Author(s): Wagenknecht, D (Wagenknecht, David); Kudrnovsky, J (Kudrnovsky, Josef); Smejkal, L (Smejkal, Libor); Carva, K (Car
Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 474 **Pages:** 517-521 **DOI:** 10.1016/j.jmmm.2018.11.047
Abstract: We investigate theoretically the combined effect of phonons and magnons caused by finite temperatures on the elect nonstoichiometric half-Heusler NiMnSb alloy. The coherent potential approximation within the alloy analogy model is employe chemical impurities, atomic displacements, and magnetic disorder. Spin fluctuations of local Mn moments are described by tw disordered local moment approach and (ii) filling of the moments.
The calculated resistivity agrees with experimental data, the agreement is good up to 600 K. We show that a strong magnetic di the Matthiessen's rule for the resistivity. We also discuss the spin polarization of the electrical current which exceeds 90% at roc dramatically reduced by the magnetic disorder for higher temperatures approaching the Curie point (T-C = 730 K).
Accession Number: WOS:000459494600076
Conference Title: 9th Joint European Magnetic Symposia (JEMS)
Conference Date: SEP 03-07, 2018
Conference Location: Mainz, GERMANY
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Wagenknecht, David	P-4165-2017	0000-0003-1927-9702
KUDRNOVSKY, Josef	G-5581-2014	0000-0002-9968-6748
Carva, Karel	A-3703-2008	0000-0002-2275-1986
Turek, Ilja	G-5553-2014	0000-0002-0604-6590

ISSN: 0304-8853
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Record 160 of 235
Title: Capturing a dynamically interacting inhibitor by paramagnetic NMR spectroscopy
Author(s): Srb, P (Srb, Pavel); Svoboda, M (Svoboda, Michal); Benda, L (Benda, Ladislav); Lepsik, M (Lepsik, Martin); Tarabek, J (Vaclav); Gruner, B (Gruener, Bohumir); Grantz-Saskova, K (Grantz-Saskova, Klara); Brynda, J (Brynda, Jiri); Rezacova, P (Rezacov (Konvalinka, Jan); Veverka, V (Veverka, Vaclav)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 21 **Issue:** 10 **Pages:** 5661-5673 **DOI:** 10.1039/c9cp00416e **Publishe**
Abstract: Transient and fuzzy intermolecular interactions are fundamental to many biological processes. Despite their importa challenging to characterize. Effects induced by paramagnetic ligands in the NMR spectra of interacting biomolecules provide an subtle manifestations of weak intermolecular interactions observed for diamagnetic ligands. Here, we present an approach to c interactions between a partially flexible dimeric protein, HIV-1 protease, and a metallacarborane-based ligand, a system for wh NMR approaches do not enable detailed structural interpretation. We show that for the case where the experimental data are si close to zero the standard fitting of pseudocontact shifts cannot provide reliable structural information. We based our approach ensemble of full atomic models, for which the experimental data can be predicted, ensemble averaged and finally compared to demonstrate that a combination of paramagnetic NMR experiments, quantum chemical calculations, and molecular dynamics towards structural characterization of dynamic protein-ligand complexes.
Accession Number: WOS:000461722800028
PubMed ID: 30794275

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Benda, Ladislav	D-8918-2011	0000-0003-4716-569X
Lepsik, Martin	X-8603-2019	0000-0003-2607-8132
Gruner, Bohumir	U-9459-2019	0000-0002-2595-9125
Srb, Pavel	C-5202-2014	0000-0002-4562-578X
Grantz Saskova, Klara	E-1931-2014	0000-0003-2874-5699
Konvalinka, Jan		0000-0003-0695-9266

ISSN: 1463-9076

eISSN: 1463-9084

Record 161 of 235

Title: Enterovirus particles expel capsid pentamers to enable genome release

Author(s): Buchta, D (Buchta, David); Fuzik, T (Fuzik, Tibor); Hrebik, D (Hrebik, Dominik); Levdansky, Y (Levdansky, Yevgen); Suk Mukhamedova, L (Mukhamedova, Liya); Moravcova, J (Moravcova, Jana); Vacha, R (Vacha, Robert); Plevka, P (Plevka, Pavel)

Source: NATURE COMMUNICATIONS **Volume:** 10 **Article Number:** 1138 **DOI:** 10.1038/s41467-019-09132-x **Published:** MAR 8 20

Abstract: Viruses from the genus Enterovirus are important human pathogens. Receptor binding or exposure to acidic pH in enc particles to an activated state that is required for genome release. However, the mechanism of enterovirus uncoating is not well cryo-electron microscopy to visualize virions of human echovirus 18 in the process of genome release. We discover that the exit of echovirus 18 results in a loss of one, two, or three adjacent capsid-protein pentamers. The opening in the capsid, which is mc enables the release of the genome without the need to unwind its putative double-stranded RNA segments. We also detect caps genome release from echovirus 30. Thus, our findings uncover a mechanism of enterovirus genome release that could become

Accession Number: WOS:000460631100023

PubMed ID: 30850609

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Vacha, Robert	M-3809-2019	
Hrebik, Dominik	M-7260-2018	0000-0003-4568-0196
Plevka, Pavel	H-8661-2014	0000-0003-4215-3315

ISSN: 2041-1723

Record 162 of 235

Title: Vibrational Optical Activity of Intermolecular, Overtone, and Combination Bands: 2-Chloropropionitrile and alpha-Pinene

Author(s): Michal, P (Michal, Pavel); Celechovsky, R (Celechovsky, Radek); Dudka, M (Dudka, Michal); Kapitan, J (Kapitan, Josef) Beresova, M (Beresova, Marie); Sebestik, J (Sebestik, Jaroslav); Thangavel, K (Thangavel, Karthick); Bour, P (Bour, Petr)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 123 **Issue:** 9 **Pages:** 2147-2156 **DOI:** 10.1021/acs.jpcb.9b00403 **Publish**

Abstract: Spectroscopy of vibrational optical activity has been established as a powerful tool to study molecular structures and only fundamental molecular transitions are analyzed. In the present study, we analyze a broader range of vibrational frequencie could be measured on a new Raman optical activity (ROA) instrument. An unexpectedly strong vibrational Raman optical activit been observed within the low-frequency region (40-150 cm(-1)). On the basis of combined molecular dynamics and density fun could be assigned to intermolecular vibrations. A detailed analysis also revealed connection between spectral shapes and mole such as bending of the CCN group. At the other edge of the scale, within similar to 1500-4000 cm(-1), for the first time, many cor bands have been observed for 2-chloropropionitrile and alpha-pinene. These were also partially assigned, using quantum-cher assignment was confirmed by a comparison with Raman, absorption, and vibrational circular dichroism spectra. The measuren vibrational range thus significantly extends the information that can be obtained by optical spectroscopy, including intermolec molecules and liquids.

Accession Number: WOS:000460996400027

PubMed ID: 30758960

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Sebestik, Jaroslav	C-9166-2012	0000-0002-0614-2064
Michal, Pavel		0000-0002-7648-6006

ISSN: 1520-6106

Record 163 of 235

Title: The complete mitogenome of Helix pomatia and the basal phylogeny of Helicinae (Gastropoda, Stylommatophora, Helici

Author(s): Korabek, O (Korabek, Ondrej); Petrusek, A (Petrusek, Adam); Rovatsos, M (Rovatsos, Michail)

Source: ZOOKEYS **Issue:** 827 **Pages:** 19-30 **DOI:** 10.3897/zookeys.827.33057 **Published:** MAR 5 2019

Abstract: A complete mitochondrial genome of the Roman snail Helix. pomatia Linnaeus, 1758 has been sequenced. The length to that of other available helicid mitogenomes. We used the mitogenome sequence to reappraise the relationships among the f groups of the helicid subfamily Helicinae. The results support the idea that the subfamily is divided between two western Palae Iberian Peninsula and western Maghreb in the west, and Anatolia, the Aegean and Caucasus in the east. One group, the tribe He and the remaining three currently recognised tribes in the west. However, the exact relationships among lineages of the non-He resolved.

Accession Number: WOS:000460299100002

PubMed ID: 31114424

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Korabek, Ondrej	P-2935-2019	0000-0002-2522-9165
Petrusek, Adam	A-3510-2008	0000-0001-5150-4370
Rovatsos, Michail T	D-3559-2013	0000-0002-8429-5680

ISSN: 1313-2989

eISSN: 1313-2970

Record 164 of 235

Title: Nitrosobenzene: Reagent for the Mitsunobu Esterification Reaction

Author(s): Pokluda, A (Pokluda, Adam); Kohout, M (Kohout, Michal); Chudoba, J (Chudoba, Josef); Krupicka, M (Krupicka, Marti

Source: ACS OMEGA **Volume:** 4 **Issue:** 3 **Pages:** 5012-5018 **DOI:** 10.1021/acsomega.8b03551 **Published:** MAR 2019

Abstract: Nitrosobenzene has been demonstrated to participate in the Mitsunobu reaction in an analogous manner to dialkyl az protocol using nitrosobenzene and triphenylphosphine (1:1) under mild conditions (0 degrees C) provides the ester derivatives acids using various alcohols in moderate yield and with good enantioselectivity, giving the desired products predominantly wit configuration. The proposed mechanism, which is analogous to that observed using dialkyl azodicarboxylates, involves a nitros triphenylphosphine adduct and an alkoxytriphenylphosphonium ion and was supported by density functional theory calculatio and experiments conducted with isotopically labeled substrates.

Accession Number: WOS:000462921900053

PubMed ID: 31459682

Author Identifiers:

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Cibulka, Radek	H-1298-2016	0000-0002-8584-7715

ISSN: 2470-1343

Record 165 of 235

Title: A review of canine B cell clonality assays and primer set optimization using large-scale repertoire data

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

Source: VETERINARY IMMUNOLOGY AND IMMUNOPATHOLOGY **Volume:** 209 **Pages:** 45-52 **DOI:** 10.1016/j.vetimm.2019.01.002 **P**

Abstract: Several molecular clonality assays have been developed to assess canine B cell proliferations. These assays were base utilized different assay designs and employed different testing strategies. This has resulted in a complex body of literature and c selection of primer sets. In addition, further refinement of primer sets is difficult because it is unknown how well current primer

sequence repertoire. The objectives of this study were 1) to provide an overview of published IGH clonality assays that highligh design and testing strategy and 2) to propose a novel method for optimizing primer sets that leverages large-scale sequencing d published assays highlighted confounding factors that hamper a direct comparison of performance metrics between studies. Tl need for a multi-institutional effort to harmonize veterinary clonality testing. A novel in silico analysis of primer sequences usin sequences identified shortfalls of existing primer sets and was used to guide primer optimization. Three optimized primer sets v qualitative sensitivity values between 80-90%. The qualitative sensitivity ranged from 1% to over 50% and was dependent on th and the sample DNA used. These findings illustrate that inclusion of high-throughput sequencing data for primer design can be design and optimization. This strategy could be applied to other antigen receptor loci or species to further improve veterinary d

Accession Number: WOS:000463294700007

PubMed ID: 30885305

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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ISSN: 0165-2427

eISSN: 1873-2534

Record 166 of 235

Title: Addressing the Compartmentalization of Specific Integrin Heterodimers in Mouse Sperm

Author(s): Frolikova, M (Frolikova, Michaela); Valaskova, E (Valaskova, Eliska); Cerny, J (Cerny, Jiri); Lumeau, A (Lumeau, Audrey Natasa); Palenikova, V (Palenikova, Veronika); Sanchez-Hernandez, N (Sanchez-Hernandez, Noemi); Pohlova, A (Pohlova, Alzbet (Manaskova-Postlerova, Pavla); Dvorakova-Hortova, K (Dvorakova-Hortova, Katerina)

Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES **Volume:** 20 **Issue:** 5 **Article Number:** 1004 **DOI:** 10.3390/ijms20 2019

Abstract: Integrins are transmembrane cell receptors involved in two crucial mechanisms for successful fertilization, namely, m signaling and cell adhesion. Integrins 64, 31 and 61 are three major laminin receptors expressed on the surface of mammalian c the presence of individual integrin subunits 3, 6, 1 and 4 has been previously detected in mammalian sperm. However, to date, individual heterodimer pairs in sperm and their detailed localization is missing. The major conclusion of this study is evidence t expressed in mouse sperm and that it pairs with subunit 6; additionally, there is a detailed identification of integrin heterodime membranes in an intact mouse sperm head. We also demonstrate the existence of 4 integrin mRNAs in round spermatids and sp which was further supported by sequencing the PCR products. Using super-resolution microscopy accompanied by colocalizati integrin subunits as follows: 6/4-inner apical acrosomal membrane and equatorial segment; 3, 6/1, 4-plasma membrane overla 3/1-outer acrosomal membrane. The existence of 64, 31 and 61 heterodimers was further confirmed by proximity ligation assay delivered detailed characterization of 3, 6, 1 and 4 integrin subunits, showing their presence in distinct compartments of the int Moreover, we identified sperm-specific localization for heterodimers 64, 31 and 61, and their membrane compartmentalization a complexity of membranes overlaying specialized microdomain structures in the sperm head. Their different protein composit membrane rafts may play a specialized role, based on their involvement in sperm-epithelium and sperm-egg interaction.

Accession Number: WOS:000462542300003

PubMed ID: 30813527

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Cerny, Jiri	I-4733-2012	0000-0002-1969-9304
Dvorakova-Hortova, Katerina	A-8705-2010	0000-0002-6837-2148
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Manaskova-Postlerova, Pavla	H-4290-2014	0000-0002-5090-4652

ISSN: 1422-0067

Record 167 of 235

Title: Modeling of Brain Tissue Heating Caused by Direct Cortical Stimulation for Assessing the Risk of Thermal Damage

Author(s): Vrba, J (Vrba, J.); Janca, R (Janca, R.); Blaha, M (Blaha, M.); Jezdik, P (Jezdik, P.); Belohlavkova, A (Belohlavkova, A.); K (Vrba, D.)

Source: IEEE TRANSACTIONS ON NEURAL SYSTEMS AND REHABILITATION ENGINEERING **Volume:** 27 **Issue:** 3 **Pages:** 440-449 **D** 10.1109/TNSRE.2019.2898253 **Published:** MAR 2019

Abstract: This paper aims to employ the numerical simulations to assess the risk of cellular damage during the application of a stimulation mapping (ESM) used in neurosurgery. The core principle of the paradigm is the use of short, high-intensity and high pulses. We developed a complex numerical model and performed coupled electro-thermal transient simulations. The model wa ESM electrodes' resistance obtained during multiple intraoperative measurements and validated by comparing them with the r distribution measurement acquired by thermal imaging. The risk of heat-induced cellular damage was assessed by applying the on the computed time-dependent spatial distribution of temperature in the brain tissue. Our results suggest that the impact of during our novel ESM paradigm is thermally non-destructive. The presented simulation results match the previously published and histopathological examination of the stimulated brain tissue and confirm the safety of the novel ESM.

Accession Number: WOS:000462435300012

PubMed ID: 30763244

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Blaha, Miroslav		0000-0001-6588-0406
Jezdik, Petr		0000-0001-8932-0497

ISSN: 1534-4320

eISSN: 1558-0210

Record 168 of 235

Title: Particle-in-cell/Monte Carlo simulation of electron and ion currents to cylindrical Langmuir probe

Author(s): Zikan, P (Zikan, Petr); Farkas, K (Farkas, Kristian); Trunec, D (Trunec, David); Jansky, J (Jansky, Jaroslav); Bonaventur

Source: CONTRIBUTIONS TO PLASMA PHYSICS **Volume:** 59 **Issue:** 3 **Pages:** 314-325 **DOI:** 10.1002/ctpp.201800063 **Published:**

Abstract: Electron and ion currents to a cylindrical Langmuir (electrostatic) probe were calculated using the particle-in-cell/Mo consistent simulation for a neutral gas in the pressure range 2-3,000 Pa. The simulation enables us to calculate the probe curren pressures when the collisions of collected charged particles with neutral gas particles near the probe are important. The main a calculation of probe currents at such high gas pressures and the comparison of the results with experimentally measured probe performed for two cases: (a) probes with varying radii in a non-thermal plasma with high electron temperature at low neutral ga verify the correctness of our simulations), and (b) probe with the radius of 10 mu m in the afterglow plasma with low electron te neutral gas pressure (up to 3,000 Pa). The electron probe currents obtained in case (a) show good agreement with those predict limited current (OMLC) theory for probes with radii up to 100 mu m for the given plasma conditions. At larger probe radii and/or OMLC theory incorrectly predicts too high an electron probe current for the plasma parameters studied. Additionally, a formula dependence of the electron density in the presheath in the collisionless case is derived. The simulation at higher neutral gas pre decrease of the electron probe current with increasing gas pressure and the creation of a large presheath around the probe. The currents are compared with those of measurements by other authors, and the differences are discussed.

Accession Number: WOS:000461229600005

ISSN: 0863-1042

eISSN: 1521-3986

Record 169 of 235

Title: The theoretical and experimental study of the Sb-Sn nano-alloys

Author(s): Kroupa, A (Kroupa, A.); Vykoukal, V (Vykoukal, V.); Kana, T (Kana, T.); Zemanova, A (Zemanova, A.); Pinkas, J (Pinkas, J

Source: CALPHAD-COMPUTER COUPLING OF PHASE DIAGRAMS AND THERMOCHEMISTRY **Volume:** 64 **Pages:** 90-96 **DOI:** 10.1016/j.calphad.2018.11.004 **Published:** MAR 2019

Abstract: The Sb-Sn nano-alloys were prepared by wet synthesis and studied experimentally and by theoretical modelling. A co ab initio method for modelling of the influence of particle size on the thermodynamic properties and phase equilibria in system phases was used to model the properties of the Sb-Sn system. The disappearance of the Sb2Sn3 phase was predicted for the ec radius below 80 nm. The experimental study carried out on Sb-Sn nanoalloys showed that Sb2Sn3 did not appear during the 1s when the morphology of sample contains agglomerates of nanoparticles with the radius below 50 nm.

Accession Number: WOS:000460842600010

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Kroupa, Ales	A-1162-2014	
Vykoukal, Vit	I-2016-2018	

ISSN: 0364-5916

eISSN: 1873-2984

Record 170 of 235

Title: Parallel colonization of subalpine habitats in the central European mountains by Primula elatior

Author(s): Konecna, V (Konecna, Veronika); Nowak, MD (Nowak, Michael D.); Kolar, F (Kolar, Filip)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 3294 **DOI:** 10.1038/s41598-019-39669-2 **Published:** MAR 1 2019

Abstract: The island-like distribution of subalpine habitats across mountain ranges can trigger the parallel evolution of locally a naturally replicated scenarios allow testing hypotheses on how elevational differentiation structures genetic diversity within sp parallel colonization of subalpine habitats across different mountain ranges has only rarely been documented with molecular d (Primulaceae), naturally spanning entire elevation range in multiple mountain regions of central Europe, to test for the origin of populations. Nuclear microsatellite variation revealed three genetic groups corresponding with the distinct study regions. We fo differentiation between foothill and subalpine populations within each region was relatively low, suggesting that the colonizati occurred independently within each mountain range. Furthermore, the strongest differentiation was usually found between the suggesting that mountain ridges may act as migration barriers that can reduce gene flow more strongly than elevational differe subalpine populations. Finally, we found that subalpine colonization did not result in a loss of genetic diversity relative to footh with the high migration rates that we document here between the subalpine and the foothill populations. In summary, our stuc elatior populations are genetically diverse and distinct results of parallel colonization events from multiple foothill gene pools.

Accession Number: WOS:000459983900100

PubMed ID: 30824749

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Konecna, Veronika	T-9822-2017	0000-0001-9568-342X

ISSN: 2045-2322

Record 171 of 235

Title: Pervasive population genomic consequences of genome duplication in Arabidopsis arenosa

Author(s): Monnahan, P (Monnahan, Patrick); Kolar, F (Kolar, Filip); Baduel, P (Baduel, Pierre); Sailer, C (Sailer, Christian); Koch, (Horvath, Robert); Laenen, B (Laenen, Benjamin); Schmickl, R (Schmickl, Roswitha); Paajanen, P (Paajanen, Pirita); Sramkova, G Bohutinska, M (Bohutinska, Magdalena); Arnold, B (Arnold, Brian); Weisman, CM (Weisman, Caroline M.); Marhold, K (Marhold, K Bomblies, K (Bomblies, Kirsten); Yant, L (Yant, Levi)

Source: NATURE ECOLOGY & EVOLUTION **Volume:** 3 **Issue:** 3 **Pages:** 457-+ **DOI:** 10.1038/s41559-019-0807-4 **Published:** MAR 2(

Abstract: Ploidy-variable species allow direct inference of the effects of chromosome copy number on fundamental evolutionar abundance of theoretical work suggests polyploidy should leave distinct population genomic signatures, empirical data remair similar to 300 individuals from 39 populations of Arabidopsis arenosa, a naturally diploidautotetraploid species. We find that th population genomic processes are subtle yet pervasive, such as reduced efficiency of purifying selection, differences in linked s flow from diploids. Initial masking of deleterious mutations, faster rates of nucleotide substitution and interploidy introgressior evolutionary potential of polyploids.

Accession Number: WOS:000459753700027

PubMed ID: 30804518

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ISSN: 2397-334X

Record 172 of 235

Title: Gallium preference for the occupation of tetrahedral sites in Lu-3(Al5-xGax)O-12 multicomponent garnet scintillators accc magnetic resonance and density functional theory calculations

Author(s): Zagorodniy, YO (Zagorodniy, Yu. O.); Chlan, V (Chlan, V.); Stepankova, H (Stepankova, H.); Fomichov, Y (Fomichov, Y.); Laguta, VV (Laguta, V. V.); Nikl, M (Nikl, M.)

Source: JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS **Volume:** 126 **Pages:** 93-104 **DOI:** 10.1016/j.jpcs.2018.10.027 **Publis**

Abstract: In this study, the distributions of aluminum and gallium atoms over the tetrahedral and octahedral sites in the garnet mixed Lu3Al5-xGaxO12 crystals by using Al-27 and Ga-71 magic angle spinning nuclear magnetic resonance (NMR) and single cr experimental study was supported by theoretical calculations based on density functional theory (DFT) in order to predict the t substitutions of Al by Ga in the mixed garnets. Both the experimental and theoretical results indicated the non-uniform distribu tetrahedral and octahedral sites in the garnet structure, with a strong preference for Ga occupying the tetrahedral sites in the ga concentrations, despite Ga having a larger ionic radius than Al and tetrahedrons being smaller than octahedrons. The Ga occup related to the involvement of Ga 3d(10) electrons in interactions, and due to the different nature of the chemical bonds formed the tetrahedral and octahedral environments. The quadrupole coupling constants and chemical shift parameters for Al and Ga r of the compounds considered, and the electric field gradients at the Al and Ga nuclei were calculated in the DFT framework. Ou structural relaxation after Al substitution with the larger Ga mainly occurs via deformation of the octahedrons, while leaving the undeformed.

Accession Number: WOS:000456224200012

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Fomichov, Yevhen		0000-0001-9002-5831
Nikl, Martin		0000-0002-2378-208X
Zagorodniy, Yuriy	S-9593-2017	0000-0002-0404-5041

ISSN: 0022-3697

eISSN: 1879-2553

Record 173 of 235

Title: Evolutionary Patterns of Thylakoid Architecture in Cyanobacteria

Author(s): Mares, J (Mares, Jan); Strunecky, O (Strunecky, Otakar); Bucinska, L (Bucinska, Lenka); Wiedermannova, J (Wiederma

Source: FRONTIERS IN MICROBIOLOGY **Volume:** 10 **Article Number:** 277 **DOI:** 10.3389/fmicb.2019.00277 **Published:** FEB 22 20

Abstract: While photosynthetic processes have become increasingly understood in cyanobacterial model strains, differences in thylakoid membranes among various lineages have been largely unexplored. Cyanobacterial cells exhibit an intriguing diversity ranging from simple parietal to radial, coiled, parallel, and special types. Although metabolic background of their variability ren suggested that thylakoid patterns are stable in certain phylogenetic clades. For decades, thylakoid arrangements have been use classification as one of the crucial characters for definition of taxa. The last comprehensive study addressing their evolutionary published 15 years ago. Since then both DNA sequence and electron microscopy data have grown rapidly. In the current study, v >200 strains onto the SSU rRNA gene tree, and the resulting phylogeny is compared to a phylogenomic tree. Changes in thylako follow the phylogeny of housekeeping loci. Parietal arrangement is resolved as the original thylakoid organization, evolving into most derived group of heterocytous cyanobacteria. Cyanobacteria occupying intermediate phylogenetic positions (greeter filar baeocytous types) exhibit fascicular, radial, and parallel arrangements, partly tracing the reconstructed course of phylogenetic previous studies, taxonomic value of thylakoid morphology seems very limited. Only special cases such as thylakoid absence or could be used as taxonomically informative apomorphies. The phylogenetic trees provide evidence of both paraphyly and rever architectures in the simple parietal thylakoid pattern. Repeated convergent evolution is suggested for the radial and fascicular a thylakoid arrangement is constrained by cell size, excluding the occurrence of complex architectures in cyanobacteria smaller t further be dependent on unknown (eco)physiological factors as suggested by recurrence of the radial type in unrelated but mor cyanobacteria, and occurrence of special features throughout the phylogeny. No straightforward phylogenetic congruences hav proteins involved in photosynthesis and thylakoid formation, and the thylakoid patterns. Remarkably, several postulated thylal partly or completely missing in cyanobacteria, challenging their proposed essential roles.

Accession Number: WOS:000459371700001

PubMed ID: 30853950

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Bucinska, Lenka	J-8858-2014	
Strunecky, Otakar	H-1629-2014	0000-0001-9735-4662

ISSN: 1664-302X

Record 174 of 235

Title: Kitaev-like honeycomb magnets: Global phase behavior and emergent effective models

Author(s): Rusnacko, J (Rusnacko, Juraj); Gotfryd, D (Gotfryd, Dorota); Chaloupka, J (Chaloupka, Jiri)

Source: PHYSICAL REVIEW B **Volume:** 99 **Issue:** 6 **Article Number:** 064425 **DOI:** 10.1103/PhysRevB.99.064425 **Published:** FEB

Abstract: Compounds of transition metal ions with strong spin-orbit coupling recently attracted attention due to the possibility dependent anisotropic magnetic interactions. In general, such interactions lead to complex phase diagrams that may include e spin liquid. Here we report on our comprehensive analysis of the global phase diagram of the extended Kitaev-Heisenberg mod lattice compounds Na(2)IrO(3)and alpha-RuCl3. We have utilized recently developed method based on spin coherent states tha arbitrary spin patterns in the cluster ground states obtained by exact diagonalization. Global trends in the phase diagram are ur with the analytical mappings of the Hamiltonian that uncover peculiar links to known models-Heisenberg, Ising, Kitaev, or com honeycomb lattice-or reveal entire manifolds of exact fluctuation-free ground states. Finally, our study can serve as a methodol applied to other spin models with complex bond-dependent non-Heisenberg interactions.

Accession Number: WOS:000459222700012

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ISSN: 2469-9950

eISSN: 2469-9969

Record 175 of 235

Title: Aromatic Azide Transformation on the Ag(111) Surface Studied by Scanning Probe Microscopy

Author(s): Hellerstedt, J (Hellerstedt, Jack); Cahlik, A (Cahlik, Ales); Stetsovych, O (Stetsovych, Oleksander); Svec, M (Svec, Mart Tomoko K.); Mutombo, P (Mutombo, Pingo); Klivar, J (Klivar, Jiri); Stara, IG (Stara, Irena G.); Jelinek, P (Jelinek, Pavel); Stary, I (S

Source: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION **Volume:** 58 **Issue:** 8 **Pages:** 2266-2271 **DOI:** 10.1002/anie.201812334

Abstract: Chemical transformation of 9-azidophenanthrene on the Ag(111) surface was studied by nc-AFM in UHV. High-resoluti first-principle calculations revealed the structure of the final products that originated from a common and elusive 9-phenanthr chemisorbed on the Ag(111) surface. A formal nitrene insertion into the C-H bond along with its dimerisation and hydrogenatio reaction channels. Thus, the ability of aryl azides to form covalent sigma- and pi-bonds between their transformation products demonstrated at a single-molecule level.

Accession Number: WOS:000458417700012

PubMed ID: 30600888

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ISSN: 1433-7851

eISSN: 1521-3773

Record 176 of 235

Title: Metal-Organic Frameworks for Helium Recovery from Natural Gas via N-2/He Separation: A Computational Screening

Author(s): Zarabadi-Poor, P (Zarabadi-Poor, Pezhman); Marek, R (Marek, Radek)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 123 **Issue:** 6 **Pages:** 3469-3475 **DOI:** 10.1021/acs.jpcc.8b07804 **Publish**

Abstract: About 500 metal-organic frameworks (MOFs) were subject to in silico screening for helium separation from natural gas helium and nitrogen was selected based on the available technical data for operating units. Geometry-based structural analysis Monte Carlo simulations was used to study several parameters including the effect of helium dilution in the gas mixture and ele target gas uptake. We established structure property relationships among various factors including adsorbent performance ind based on their performance which also brought us valuable knowledge on the desired ranges of helium void fraction, accessibl diameter. We have identified top 10 performing MOFs for adsorption-based separation which have been consequently studied i deeper insight on the possible adsorption sites and adsorptive behavior. We also assessed the diffusion-based separation to ide based on membrane selectivity.

Accession Number: WOS:000459223200074

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
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Zarabadi-Poor, Pezhman	A-6362-2011	0000-0002-6377-7592

ISSN: 1932-7447

Record 177 of 235

Title: Toward Ab Initio Protein Folding: Inherent Secondary Structure Propensity of Short Peptides from the Bioinformatics and Perspective

Author(s): Culka, M (Culka, Martin); Galgonek, J (Galgonek, Jakub); Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri); Ru

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 123 **Issue:** 6 **Pages:** 1215-1227 **DOI:** 10.1021/acs.jpcb.8b09245 **Publish**

Abstract: By combining bioinformatics with quantum-chemical calculations, we attempt to address quantitatively some of the protein folding. The former allowed us to identify tripeptide sequences in existing protein three-dimensional structures with a s helical or extended structure. The selected representatives of pro-helical and pro-extended sequences were converted into "iso N- and C-termini-and these were subjected to an extensive conformational sampling and geometry optimization (typically thou conformers for each tripeptide). For each conformer, the QM(DFT-D3)/COSMO-RS free-energy value was then calculated, G(conf (solv) is expected to provide an objective, unbiased, and quantitatively accurate measure of the conformational preference of tl sequence. It has been shown that irrespective of the helical vs extended preferences of the selected tripeptide sequences in cor the low-energy conformers of isolated tripeptides prefer the R-helical structure. Nevertheless, pro-helical tripeptides show sligh than their pro-extended counterparts. Furthermore, when the sampling is repeated in the presence of a partner tripeptide to m sheet, pro-extended tripeptides (exemplified by the VIV) show a larger free-energy benefit than pro-helical tripeptides (exempli even more pronounced in a hydrophobic solvent, which mimics the less polar parts of a protein. This is in line with our bioinfor majority of pro-extended tripeptides are hydrophobic. The preference for a specific secondary structure by the studied tripepti plasticity to adopt to its environment. In addition, we show that most of the "naturally occurring" conformations of tripeptide s existing three-dimensional protein structures, are within similar to 10 kcal.mol(-1) from their global minima. In summary, our "a complex protein structures may start to emerge already at the level of their small oligopeptidic units, which is in line with a hier folding.

Accession Number: WOS:000459223800001

PubMed ID: 30645123

Author Identifiers:

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ISSN: 1520-6106

Record 178 of 235

Title: Acidogenesis, solventogenesis, metabolic stress response and life cycle changes in Clostridium beijerinckii NRRL B-598 at

Author(s): Patakova, P (Patakova, Petra); Branska, B (Branska, Barbora); Sedlar, K (Sedlar, Karel); Vasylkivska, M (Vasylkivska, M (Jureckova, Katerina); Kolek, J (Kolek, Jan); Koscova, P (Koscova, Pavlina); Provaznik, I (Provaznik, Ivo)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 1371 **DOI:** 10.1038/s41598-018-37679-0 **Published:** FEB 4 2019

Abstract: Clostridium beijerinckii NRRL B-598 is a sporulating, butanol and hydrogen producing strain that utilizes carbohydrat ethanol (ABE) fermentative pathway. The pathway consists of two metabolic phases, acidogenesis and solventogenesis, from w coupled with sporulation. Thorough transcriptomic profiling during a complete life cycle and both metabolic phases completec microscopy and a metabolites analysis helped to find out key genes involved in particular cellular events. The description of ge involved in metabolism or the cell cycle is a necessary condition for metabolic engineering of the strain and will be valuable for other Clostridial species. The study focused on glucose transport and catabolism, hydrogen formation, metabolic stress respon motility/chemotaxis and sporulation, which resulted in the composition of the unique image reflecting clostridial population ch change in expression of individual genes was coupled with the sporulation start and not with the transition from acidogenic to s expected, solvents formation started at pH decrease and the accumulation of butyric and acetic acids in the cultivation mediun

Accession Number: WOS:000457616300259

PubMed ID: 30718562

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Branska, Barbora	G-6429-2019	0000-0001-6536-7063

ISSN: 2045-2322

Record 179 of 235

Title: Low-Cycle Fatigue, Fractography and Life Assessment of EN AW 2024-T351 under Various Loadings

Author(s): Pec, M (Pec, M.); Zapletal, J (Zapletal, J.); Sebek, F (Sebek, F.); Petruska, J (Petruska, J.)

Source: EXPERIMENTAL TECHNIQUES **Volume:** 43 **Issue:** 1 **Pages:** 41-56 **DOI:** 10.1007/s40799-018-0263-0 **Published:** FEB 201

Abstract: The paper provides extensive experiments on aluminium alloy 2024-T351. Those cover the uniaxial strain- and stress- cylindrical specimens. Then, multiaxial tests were conducted via strain- and stress-controlled tensile-torsional loading on tubul cover the followingnon-proportional test - the 3-step experiment carried out in order to document the additional hardening. Th fractography using the scanning electron microscopy and the life assessment. A novel approach to fatigue life prediction is pres plastic part of the strain-life curve by the non-linear term in order to provide more variability and approximation ability. The bro serve as a basis for future calibration and simulation using advanced cyclic plasticity models within the finite elements.

Accession Number: WOS:000466234600005

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Sebek, Frantisek	I-5694-2013	0000-0003-3813-6555

ISSN: 0732-8818

eISSN: 1747-1567

Record 180 of 235

Title: Selective -N-acetylhexosaminidase from Aspergillus versicolora tool for producing bioactive carbohydrates

Author(s): Bojarova, P (Bojarova, Pavla); Kulik, N (Kulik, Natallia); Slamova, K (Slamova, Kristyna); Hubalek, M (Hubalek, Martin) Cvacka, J (Cvacka, Josef); Pelantova, H (Pelantova, Helena); Kren, V (Kren, Vladimir)

Source: APPLIED MICROBIOLOGY AND BIOTECHNOLOGY **Volume:** 103 **Issue:** 4 **Pages:** 1737-1753 **DOI:** 10.1007/s00253-018-953

Abstract: -N-Acetylhexosaminidases (EC 3.2.1.52) are typical of their dual activity encompassing both N-acetylglucosamine and substrates. Here we present the isolation and characterization of a selective -N-acetylhexosaminidase from the fungal strain of A enzyme was recombinantly expressed in Pichia pastoris KM71H in a high yield and purified in a single step using anion-exchang Homologous molecular modeling of this enzyme identified crucial differences in the enzyme active site that may be responsible N-acetylglucosamine substrates compared to fungal -N-acetylhexosaminidases from other sources. The enzyme was used in a s with a mutant -N-acetylhexosaminidase from Talaromyces flavus with an enhanced synthetic capability, affording a bioactive d functional group. The azido function enabled an elegant multivalent presentation of this disaccharide on an aromatic carrier. T glycoconjugate is applicable as a selective ligand of galectin-3a biomedically attractive human lectin. These results highlight th availability of robust and well-defined carbohydrate-active enzymes with tailored catalytic properties for biotechnological and

Accession Number: WOS:000459250200016

PubMed ID: 30603849

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Kulik, Natalia	AAC-4283-2019	0000-0003-2005-8165
Bojarova, Pavla	R-4742-2017	0000-0001-7069-0973

ISSN: 0175-7598

eISSN: 1432-0614

Record 181 of 235

Title: Sperm divergence in a passerine contact zone: Indication of reinforcement at the gametic level

Author(s): Albrecht, T (Albrecht, Tomas); Opletalova, K (Opletalova, Kamila); Reif, J (Reif, Jiri); Janousek, V (Janousek, Vaclav); F Cramer, ERA (Cramer, Emily R. A.); Johnsen, A (Johnsen, Arild); Reifova, R (Reifova, Radka)

Source: EVOLUTION **Volume:** 73 **Issue:** 2 **Pages:** 202-213 **DOI:** 10.1111/evo.13677 **Published:** FEB 2019

Abstract: Postcopulatory sexual selection may promote evolutionary diversification in sperm form, but the contribution of betv sperm morphology to the origin of reproductive isolation and speciation remains little understood. To assess the possible role reproductive isolation, we studied sperm morphology in two closely related bird species, the common nightingale (Luscinia me nightingale (Luscinia luscinia), that hybridize in a secondary contact zone spanning Central and Eastern Europe. We found: (1) s the species in total sperm length, accompanied by a difference in the length of the mitochondrial sperm component; (2) greate in sperm morphology in sympatry than in allopatry, with evidence for character displacement in sperm head length detected in interspecific hybrids showing sperm with a length intermediate between the parental species, but no evidence for decreased sp of abnormal spermatozoa in ejaculates). Our results demonstrate that divergence in sperm morphology between the two night in intrinsic postzygotic isolation, but may contribute to postcopulatory prezygotic isolation. This isolation could be strengthene reinforcement.

Accession Number: WOS:000458847800006

PubMed ID: 30597549

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Reifova, Radka	D-2137-2011	0000-0001-5852-5174
Albrecht, Tomas	A-1130-2011	
Pialek, Lubomir	G-4611-2015	0000-0003-1881-4646
Reif, Jiri	I-9168-2017	0000-0003-2553-7333
Albrecht, Tomas		0000-0002-9213-0034

ISSN: 0014-3820

eISSN: 1558-5646

Record 182 of 235

Title: Probing the Accuracy of First-Principles Modeling of Molecular Crystals: Calculation of Sublimation Pressures

Author(s): Cervinka, C (Cervinka, Ctirad); Fulem, M (Fulem, Michal)

Source: CRYSTAL GROWTH & DESIGN **Volume:** 19 **Issue:** 2 **Pages:** 808-820 **DOI:** 10.1021/acs.cgd.8b01374 **Published:** FEB 2019

Abstract: An insight into current possibilities of obtaining the sublimation pressures for molecular crystals from first principles extreme sensitivity to any computational uncertainties, sublimation pressures are the strictest possible representation of first-p properties of molecular crystals, emphasizing the significance of any computational uncertainties of cohesive energies, sublim sublimation entropies which might seem acceptable from a purely energetic point of view. The sublimation pressure was comp molecular crystals by combining the calculated static cohesive energy, vibrational contributions to thermodynamic properties ideal-gas thermodynamic properties required to obtain the sublimation enthalpy and entropy as a function of temperature. Th pressures were compared to reference experimentally based values developed in this work. By an analysis of the uncertainties to experimental sublimation pressures and both enthalpic and entropic contributions, the uncertainty limits for prediction of su first-principles approaches are discussed and estimated. As the sublimation pressure depends exponentially on both enthalpic the current accuracy of first-principles calculations allows its prediction typically within a factor of 10. This can still be viewed a uncertainties in experimentally determined sublimation thermodynamic properties, especially when extremely low volatility co

Accession Number: WOS:000458348000035

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Fulem, Michal	B-7450-2008	0000-0002-5707-0670

ISSN: 1528-7483

eISSN: 1528-7505

Record 183 of 235

Title: Novel quinazolin-4-one derivatives as potentiating agents of doxorubicin cytotoxicity

Author(s): Pospisilova, M (Pospisilova, Monika); Andrs, M (Andrs, Martin); Seifrtova, M (Seifrtova, Martina); Havelek, R (Havelek, Tomsik, P (Tomsik, Pavel); Prchal, L (Prchal, Lukas); Dolezal, R (Dolezal, Rafael); Tichy, A (Tichy, Ales); Kucera, T (Kucera, Tomas); Jan); Rezacova, M (Rezacova, Martina)

Source: BIOORGANIC CHEMISTRY **Volume:** 82 **Pages:** 204-210 **DOI:** 10.1016/j.bioorg.2018.10.001 **Published:** FEB 2019

Abstract: We report the design, synthesis and biological evaluation of 17 novel 8-aryl-2-morpholino-3,4-dihydroquinazoline de standard model of DNA-PK and PI3K inhibitors. Novel compounds are sub-divided into two series where the second series of fiv have a better solubility profile over the first one. A combination of in vitro and in silico techniques suggested a plausible synergi the most potent compound 14d on cell proliferation via DNA-PK and poly(ADP-ribose) polymerase-1 (PARP-1) inhibition, while a effect on cell proliferation.

Accession Number: WOS:000455479600022

PubMed ID: 30326402

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rezacova, Martina	A-2046-2009	0000-0001-5370-2290
Prchal, Lukas		0000-0001-9698-4478

ISSN: 0045-2068

eISSN: 1090-2120

Record 184 of 235

Title: Interaction of Chiral and Achiral Dimethylsuccinic Acid Diastereomers with a Cu(110) Surface

Author(s): Karageorgaki, C (Karageorgaki, Chrysanthi); Mutombo, P (Mutombo, Pingo); Ernst, KH (Ernst, Karl-Heinz)

Source: JOURNAL OF PHYSICAL CHEMISTRY C **Volume:** 123 **Issue:** 4 **Pages:** 2329-2335 **DOI:** 10.1021/acs.jpcc.8b11320 **Publish**

Abstract: The transmission of chirality to an achiral metal surface after adsorption of chiral or achiral molecules is an exciting ap systems. The interaction of racemic 2,3-dimethylsuccinic acid and its achiral meso form with a Cu(110) surface has been investi means of X-ray photoelectron spectroscopy, low-energy electron diffraction, reflection absorption infrared spectroscopy, scann temperature-programmed desorption, and density functional theory. Racemic as well as meso-2,3-dimethylsuccinic acid form structures, coexisting with extended two-dimensional structures that do not break the mirror symmetry of the substrate surface the molecules suggest a chiral reconstruction of the surface. The thermally induced decomposition proceeds autocatalytically i explosion and shows a profound difference for the diastereomers.

Accession Number: WOS:000457816600033

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Mutombo, Pingo	G-5266-2014	0000-0002-8175-7587

ISSN: 1932-7447

Record 185 of 235

Title: Evolution of sex determination and heterogamety changes in section Otites of the genus Silene

Author(s): Balounova, V (Balounova, Veronika); Gogela, R (Gogela, Roman); Cegan, R (Cegan, Radim); Cangren, P (Cangren, Patr Jitka); Safar, J (Safar, Jan); Kovacova, V (Kovacova, Viera); Bergero, R (Bergero, Roberta); Hobza, R (Hobza, Roman); Vyskot, B (Vy (Oxelman, Bengt); Charlesworth, D (Charlesworth, Deborah); Janousek, B (Janousek, Bohuslav)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 1045 **DOI:** 10.1038/s41598-018-37412-x **Published:** JAN 31 2019

Abstract: Switches in heterogamety are known to occur in both animals and plants. Although plant sex determination systems recently than those in several well-studied animals, including mammals, and have had less time for switches to occur, we previ heterogamety in the plant genus Silene: section Otites has both female and male heterogamety, whereas S. latifolia and its clos section of the genus, Melandrium (subgenus Behenantha), all have male heterogamety. Here we analyse the evolution of sex ch

which is estimated to have evolved only about 0.55 MYA. Our study confirms female heterogamety in S. otites and newly reveals borysthenica. Sequence analyses and genetic mapping show that the sex-linked regions of these two species are the same, but close relative with male heterogamety, is different. The sex chromosome pairs of S. colpophylla and S. otites each correspond t species, and both differ from the XY pair in S. latifolia. Silene section Otites species are suitable for detailed studies of the event and our phylogenetic analysis suggests a possible change from female to male heterogamety within this section. Our analyses s so far not been considered, change in heterogamety through hybridization, in which a male-determining chromosome from on another one, and over-rides its previous sex-determining system.

Accession Number: WOS:000457287000033

PubMed ID: 30705300

ISSN: 2045-2322

Record 186 of 235

Title: Microscopic multiphonon approach to nuclei with a valence hole in the oxygen region

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

Source: PHYSICAL REVIEW C **Volume:** 99 **Issue:** 1 **Article Number:** 014316 **DOI:** 10.1103/PhysRevC.99.014316 **Published:** JAN 2

Abstract: An equation of motion phonon method, developed for even nuclei and recently extended to odd systems with a valen the hole-phonon coupling scheme and applied to A = 15 and A = 21 isobars with a valence hole. The method derives a set of equ orthonormal basis of states composed of a hole coupled to an orthonormal basis of correlated n-phonon states (n = 0, 1, 2, . . .), Dancoff phonons, describing the excitations of a doubly magic core. The basis is then adopted to solve the full eigenvalue probl exact but lends itself naturally to simplifying approximations. Self-consistent calculations using a chiral Hamiltonian in a space phonon and three-phonon basis states in A = 21 and A = 15 nuclei, respectively, yield full spectra, moments, electromagnetic an strengths, and electric dipole cross sections. The analysis of the hole-phonon composition of the eigenfunctions contributes to excitation of levels and resonances and to understand the reasons of the deviations of the theory from the experiments. Prescri discrepancies are suggested.

Accession Number: WOS:000456777600001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
De Gregorio, Giovanni	AAH-2437-2019	0000-0003-0253-915X
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290

ISSN: 2469-9985

eISSN: 2469-9993

Record 187 of 235

Title: Sperm-dependent asexual hybrids determine competition among sexual species

Author(s): Janko, K (Janko, Karel); Eisner, J (Eisner, Jan); Mikulicek, P (Mikulicek, Peter)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 722 **DOI:** 10.1038/s41598-018-35167-z **Published:** JAN 24 2019

Abstract: Interspecific competition is a fundamental process affecting community structure and evolution of interacting specie this process is also mediated by shared enemies, which can change the outcome of competition dramatically. However, previou interactions between competing species and their parasites (parasite-mediated competition) completely overlooked the effect sperm-dependent parthenogens or pseudogams) on competition. These organisms originate by interspecific hybridization, pro exploit parental species for their own reproduction, being therefore analogous to classical parasites. Here we use the reaction-d pseudogams alter the outcome of interspecific competition significantly. They may either slow down competitive exclusion of t turn the outcome of competition between the species. Asexual organisms may thus have unexpectedly strong impact on comm more significant evolutionary potential than was previously thought.

Accession Number: WOS:000456554600161

PubMed ID: 30679449

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Mikulicek, Peter	AAD-1684-2019	

ISSN: 2045-2322

Record 188 of 235

Title: Detailed characterization of the Arthrospira type species separating commercially grown taxa into the new genus Limnosp

Author(s): Nowicka-Krawczyk, P (Nowicka-Krawczyk, Paulina); Muhlsteinova, R (Muhlsteinova, Radka); Hauer, T (Hauer, Tomas)

Source: SCIENTIFIC REPORTS **Volume:** 9 **Article Number:** 694 **DOI:** 10.1038/s41598-018-36831-0 **Published:** JAN 24 2019

Abstract: The genus Arthrospira has a long history of being used as a food source in different parts of the world. Its mass cultiva supplements and additives has contributed to a more detailed study of several species of this genus. In contrast, the type speci has scarcely been studied. This work adopts a polyphasic approach to thoroughly investigate environmental samples of A. jenn was noticed in an urban reservoir in Poland, Central Europe. The obtained results were compared with strains designated as A. fusiformis from several culture collections and other Arthrospira records from GenBank. The comparison has shown that A. jenr species that are massively utilized commercially with regard to its cell morphology, ultrastructure and ecology, as well as its 16 on our findings, we propose the establishment of a new genus, Limnospira, which currently encompasses three species includi (A.) fusiformis and L. (A.) maxima with the type species Limnospira fusiformis.

Accession Number: WOS:000456554600133

PubMed ID: 30679537

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Hauer, Tomas	F-5089-2010	0000-0002-8005-5874

ISSN: 2045-2322

Record 189 of 235

Title: Crossover in the inelastic electron tunneling spectra of conjugated molecules with direct Au-C links

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

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS **Volume:** 21 **Issue:** 3 **Pages:** 1564-1571 **DOI:** 10.1039/c8cp06290k **Published**

Abstract: We use inelastic electron tunneling spectroscopy (IETS) first-principles simulations to identify and characterize the dif single conjugated molecules bonded to Au metal electrodes. The molecules are polyphenyls (with 1 to 4 benzene units) bonded direct Au-C bonds. The short molecule shows near resonant elastic transmission, with a crossover to tunneling for the longer ba inelastic spectra exhibit dips in the IETS signal of the short molecule and peaks for the longer molecules. We characterize the sy and scattering states and discuss the changes with increasing length, where the inelastic signal of different modes can be ampli crossover as more benzene units are added to the molecular backbone. This analysis rationalizes the observed trends as a func illustrates the role of electronic and vibrational properties on Au-C bonded molecular junctions.

Accession Number: WOS:000456147000063

PubMed ID: 30620028

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Foti, Giuseppe	R-9835-2019	0000-0001-5769-2253
Vazquez, Hector	G-5788-2014	0000-0002-3865-9922

ISSN: 1463-9076

eISSN: 1463-9084

Record 190 of 235

Title: The interaction of proteins with silica surfaces. Part II: Free energies of capped amino acids

Author(s): Trachta, M (Trachta, Michal); Bludsky, O (Bludsky, Ota); Rubes, M (Rubes, Miroslav)

Source: COMPUTATIONAL AND THEORETICAL CHEMISTRY **Volume:** 1148 **Pages:** 38-43 **DOI:** 10.1016/j.comptc.2018.12.013 **Pub**

Abstract: Binding free energies of the fifteen proteinogenic amino acids were investigated for neutral silica surfaces of varying s biased molecular dynamics. A new force field parameterized to reproduce the results of highly accurate ab initio calculations ha simulations to provide a balanced description of the adsorbate silica interactions. The calculated free energies increase in the o IPC-1P. The surface heterogeneity and the local curvature enhance the binding free energy due to the cooperative effects betwe hydrophobic and hydrophilic parts of amino acids. The propensity towards amino acids with aromatic side chains has been obs surfaces, with the effect being much stronger for the quartz without surface silanol groups than for fully hydroxylated silica surf

Accession Number: WOS:000458595400006

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Bludsky, Ota	A-5659-2008	0000-0001-5366-3586
Trachta, Michal	G-8118-2014	0000-0001-5084-3434

ISSN: 2210-271X
eISSN: 1872-7999

Record 191 of 235

Title: AmtDB: a database of ancient human mitochondrial genomes

Author(s): Ehler, E (Ehler, Edvard); Novotny, J (Novotny, Jiri); Juras, A (Juras, Anna); Chylenski, M (Chylenski, Maciej); Moravcik, (Paces, Jan)

Source: NUCLEIC ACIDS RESEARCH **Volume:** 47 **Issue:** D1 **Pages:** D29-D32 **DOI:** 10.1093/nar/gky843 **Published:** JAN 8 2019

Abstract: Ancient mitochondrial DNA is used for tracing human past demographic events due to its population-level variability. ancient mitochondrial genomes has increased in recent years, alongside with the development of high-throughput sequencing methods. Here, we present AmtDB, the first database of ancient human mitochondrial genomes. Release version contains 1107 samples, freely accessible for download, together with the individual descriptors, including geographic location, radiocarbon d culture affiliation. The database also features an interactive map for sample location visualization. AmtDB is a key platform for a studies and is available at https://amtdb.org.

Accession Number: WOS:000462587400005
PubMed ID: 30247677

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Novotny, Jiri	S-6426-2019	0000-0003-1338-638X
Paces, Jan	C-8851-2009	0000-0003-3059-6127
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Ehler, Edvard		0000-0001-6212-6301
Chylenski, Maciej		0000-0003-1347-1904

ISSN: 0305-1048
eISSN: 1362-4962

Record 192 of 235

Title: Computational Study of Protein-Ligand Unbinding for Enzyme Engineering

Author(s): Marques, SM (Marques, Sergio M.); Bednar, D (Bednar, David); Damborsky, J (Damborsky, Jiri)

Source: FRONTIERS IN CHEMISTRY **Volume:** 6 **Article Number:** 650 **DOI:** 10.3389/fchem.2018.00650 **Published:** JAN 8 2019

Abstract: The computational prediction of unbinding rate constants is presently an emerging topic in drug design. However, the kinetic rates is not restricted to pharmaceutical applications. Many biotechnologically relevant enzymes have their efficiency lir substrates or the release of products. While aiming at improving the ability of our model enzyme haloalkane dehalogenase Dha anthropogenic pollutant 1,2,3-trichloropropane (TCP), the DhaA31 mutant was discovered. This variant had a 32-fold improvem toward TCP, but the catalysis became rate-limited by the release of the 2,3-dichloropropan-1-ol (DCP) product from its buried a computational study to estimate the unbinding rates of the products from DhaA and DhaA31. The metadynamics and adaptive s to predict the relative order of kinetic rates in the different systems, while the absolute values depended significantly on the co field, and water model). Free energy calculations provided the energetic landscape of the unbinding process. A detailed analysi energetic bottlenecks allowed the identification of the residues playing a key role during the release of DCP from DhaA31 via th these hot-spots could also be identified by the fast CaverDock tool for predicting the transport of ligands through tunnels. Targe mutagenesis should improve the unbinding rates of the DCP product and the overall catalytic efficiency with TCP.

Accession Number: WOS:000455109700001
PubMed ID: 30671430

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Marques, Sergio M	H-8685-2012	0000-0002-6281-7505
Bednar, David		0000-0002-6803-0340

ISSN: 2296-2646

Record 193 of 235

Title: Forward dihadron back-to-back correlations in pA collisions

Author(s): Albacete, JL (Albacete, Javier L.); Giacalone, G (Giacalone, Giuliano); Marquet, C (Marquet, Cyrille); Matas, M (Matas, M

Source: PHYSICAL REVIEW D **Volume:** 99 **Issue:** 1 **Article Number:** 014002 **DOI:** 10.1103/PhysRevD.99.014002 **Published:** JAN

Abstract: We study the disappearance of the away-side peak of the di-hadron correlation function in p + A vs p + p collisions at f scaterring process presents a manifest dilute-dense asymmetry. We improve the state-of-the-art description of this phenomenc color glass condensate (CGC), for hadrons produced nearly back to back. In that case, the gluon content of the saturated nuclea transverse-momentum-dependent gluon distributions, whose small-x evolution we calculate numerically by solving the Balitsk running coupling corrections. We first show that our formalism provides a good description of the disappearance of the away-si + Au collisions observed at BNL Relativistic Heavy Ion Collider (RHIC) energies. Then, we predict the away-side peak of upcomin GeV to be suppressed by about a factor 2 with respect to p + p collisions, and we propose to study the rapidity dependence of th complementary strong evidence of gluon saturation in experimental data.

Accession Number: WOS:000454768700002

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Lopez Albacete, Javier	D-9272-2016	0000-0001-8345-6123

ISSN: 2470-0010

eISSN: 2470-0029

Record 194 of 235

Title: Structural Biology and Protein Engineering of Thrombolytics

Author(s): Mican, J (Mican, Jan); Toul, M (Toul, Martin); Bednar, D (Bednar, David); Damborsky, J (Damborsky, Jiri)

Source: COMPUTATIONAL AND STRUCTURAL BIOTECHNOLOGY JOURNAL **Volume:** 17 **Pages:** 917-938 **DOI:** 10.1016/j.csbj.2019

Abstract: Myocardial infarction and ischemic stroke are the most frequent causes of death or disability worldwide. Due to their the thrombolytics are frequently used for their treatment. Improving the effectiveness of thrombolytics for clinical uses is of gre the multiple roles of the endogenous thrombolytics and the fibrinolytic system grows continuously. The effects of thrombolytic nervous system and the regulation of the cell migration offer promising novel uses for treating neurodegenerative disorders or t However, secondary activities of thrombolytics may lead to life-threatening side-effects such as intracranial bleeding and neurc structural biology perspective on various thrombolytic enzymes and their key properties: (i) effectiveness of clot lysis, (ii) affinit fibrin, (iii) biological half-life, (iv) mechanisms of activation/inhibition, and (v) risks of side effects. This information needs to be establishing protein engineering strategies aiming at the development of novel thrombolytics. Current trends and perspectives screening for novel enzymes and small molecules, the enhancement of fibrin specificity by protein engineering, the suppressio receptors, liposomal encapsulation and targeted release, the application of adjuvants, and the development of improved produ

Accession Number: WOS:000504205700091

PubMed ID: 31360331

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Bednar, David		0000-0002-6803-0340

ISSN: 2001-0370

Record 195 of 235

Title: FPGA Packet Reflector for Network Path Testing

Author(s): Ubik, S (Ubik, Sven); Hynek, K (Hynek, Karel); Melnikov, J (Melnikov, Jiri)

Edited by: RimacDrlje S; Zagar D; Galic I; Martinovic G; Vranjes D; Habijan M

Source: PROCEEDINGS OF 2019 INTERNATIONAL CONFERENCE ON SYSTEMS, SIGNALS AND IMAGE PROCESSING (IWSSIP 2019) Conference on Systems Signals and Image Processing **Pages:** 39-42 **Published:** 2019

Abstract: Testing of a network path for suitability for demanding network applications can be assisted by using a packet reflecto packets generated by a network application across a network and back to the source where they are received by the applicatior observed. We propose the design of a high-performance hardware accelerated packet reflector, compare its performance chara solutions and give recommendations for practical use.

Accession Number: WOS:000501745100005

Conference Title: 26th International Conference on Systems, Signals and Image Processing (IWSSIP)

Conference Date: JUN 05-07, 2019

Conference Location: Josip Juraj Strossmayer Univ Osijek, Fac Elect Engn, Comp Sci & Informat T, Osijek, CROATIA

Conference Sponsors: European Assoc Signal Proc, IEEE Croatia Sect, Commun Chapter, Syst Man & Cybernet Chapter, Reliabil Croatian Acad Engn

Conference Host: Josip Juraj Strossmayer Univ Osijek, Fac Elect Engn, Comp Sci & Informat T
ISSN: 2157-8672
ISBN: 978-1-7281-3227-3

Record 196 of 235

Title: Visual Analysis of Ligand Trajectories in Molecular Dynamics

Author(s): Jurcik, A (Jurcik, Adam); Furmanova, K (Furmanova, Katarina); Byska, J (Byska, Jan); Vonasek, V (Vonasek, Vojtech); V
Ulbrich, P (Ulbrich, Pavol); Hauser, H (Hauser, Helwig); Kozlikova, B (Kozlikova, Barbora)

Edited by: Maciejewski R; Seo J; Westermann R

Source: 2019 IEEE PACIFIC VISUALIZATION SYMPOSIUM (PACIFICVIS 2019) **Book Series:** IEEE Pacific Visualization Symposium **P**
10.1109/PacificVis.2019.00032 **Published:** 2019

Abstract: In many cases, protein reactions with other small molecules (ligands) occur in a deeply buried active site. When study
is crucial for biochemists to examine trajectories of ligand motion. These trajectories are predicted with in-silico methods that p
possible trajectories. In this paper, we propose a novel approach to the interactive visual exploration and analysis of large sets o
the domain experts to understand protein function based on the trajectory properties. The proposed solution is composed of m
views, enabling the interactive exploration and filtering of trajectories in an informed way. In the workflow, we focus on the pra
interactive visual analysis specific to ligand trajectories. We adapt the small multiples principle to resolve an overly large numb
chunks that are easier to analyze. We describe how drill-down techniques can be used to create and store selections of the traje
properties, enabling the comparison of multiple datasets. In appropriately designed 2D and 3D views, biochemists can either ol
or choose to aggregate the information into a functional boxplot or density visualization. Our solution is based on a tight collab
experts, aiming to address their needs as much as possible. The usefulness of our novel approach is demonstrated by two case
collaborating protein engineers.

Accession Number: WOS:000502097000020
Conference Title: 12th IEEE Pacific Visualization Symposium (IEEE PacificVis)
Conference Date: APR 23-26, 2019
Conference Location: Chulalongkorn Univ, Bangkok, THAILAND
Conference Sponsors: IEEE, IEEE Comp Soc, IEEE Comp Soc, Visualizat & Graph Tech Comm
Conference Host: Chulalongkorn Univ
ISSN: 2165-8765
ISBN: 978-1-5386-9226-4

Record 197 of 235

Title: Development and deployment of the main parts of LoRaWAN private network

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

Edited by: Dudzik MC; Ricklin JC

Source: AUTONOMOUS SYSTEMS: SENSORS, PROCESSING, AND SECURITY FOR VEHICLES AND INFRASTRUCTURE 2019 **Book Se**
SPIE **Volume:** 11009 **Article Number:** UNSP 110090F **DOI:** 10.1117/12.2518225 **Published:** 2019

Abstract: The significant expansion of the Internet of Things (IoT) field and unique requirements of the IoT devices bring new te
exclusively to provide wireless connectivity for the IoT devices. Among these technologies, we can include LoRa technology. Un
LoRa technology is an open standard, and it allows us to build private networks. We took advantage of that and developed our
a proposal of network infrastructure and the hardware solution of the LoRaWAN gateway based on the second generation of mo
Raspberry Pi model B and fully compatible LoRaWAN 868 MHz iC880A concentrator. The concentrator is connected to Raspberry
Interface (SPI). In 2018, five gateways were deployed to cover a nearly entire area of Ostrava city in the Czech Republic and its su
LoRaWAN signal. Our solution uses The Things Network platform to connect to a global open crowd-sourced IoT data network.
implemented a web application that serves as a backend for registration of the end-devices to the LoRaWAN network, and it pro
all uplink messages transmitted by end-devices and received by LoRaWAN network. The next part of the article discusses end-d
availability testing.

Accession Number: WOS:000502029400009
Conference Title: Conference on Autonomous Systems - Sensors, Processing, and Security for Vehicles and Infrastructure
Conference Date: APR 15-16, 2019
Conference Location: Baltimore, MD
Conference Sponsors: SPIE
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Safarik, Jakub		0000-0002-3360-2302

ISSN: 0277-786X
eISSN: 1996-756X
ISBN: 978-1-5106-2684-3

Record 198 of 235

Title: Betatron radiation enhancement by a density up-ramp in the bubble regime of LWFA

Author(s): Maslarova, D (Maslarova, Dominika); Horny, V (Horny, Vojtech); Krus, M (Krus, Miroslav); Psikal, J (Psikal, Jan)

Edited by: Esarey E; Schroeder CB; Schreiber J

Source: LASER ACCELERATION OF ELECTRONS, PROTONS, AND IONS V **Book Series:** Proceedings of SPIE **Volume:** 11037 **Articl** 1103710 **DOI:** 10.1117/12.2520980 **Published:** 2019

Abstract: We examine betatron radiation properties from the bubble regime of laser-wakefield acceleration for a tailored plasm studies have already discussed enhancement of radiation properties by using various density modifications in later acceleratio on a density profile with a short linear up-ramp and compare it with a uniform density case. The process is studied for standard current sub-100 TW laser systems by means of numerical particle-in-cell simulations. We show here that the critical energy and when the plasma density increases. This enhancement is caused either by electron energy gain in the rear part of the bubble or boost by fields behind the bubble.

Accession Number: WOS:000502118100010

Conference Title: Conference on Laser Acceleration of Electrons, Protons, and Ions V

Conference Date: APR 01-03, 2019

Conference Location: Prague, CZECH REPUBLIC

Conference Sponsors: SPIE

ISSN: 0277-786X

eISSN: 1996-756X

ISBN: 978-1-5106-2741-3

Record 199 of 235

Title: Comparison of ion acceleration from nonexpanded and expanded thin foils irradiated by ultrashort petawatt laser pulse

Author(s): Psikal, J (Psikal, J.); Horny, V (Horny, V); Zakova, M (Zakova, M.); Matys, M (Matys, M.)

Edited by: Esarey E; Schroeder CB; Schreiber J

Source: LASER ACCELERATION OF ELECTRONS, PROTONS, AND IONS V **Book Series:** Proceedings of SPIE **Volume:** 11037 **Articl** 1103708 **DOI:** 10.1117/12.2520278 **Published:** 2019

Abstract: It is usually assumed that ions are accelerated most efficiently in the case of non-expanded targets irradiated by femt pulse, alternatively with only short scale preplasma on their front side. Here, we demonstrate that the ions in an expanded foil plasma before its interaction with the main petawatt pulse may be accelerated to higher energies than that from ultrathin foils. mechanisms responsible for the acceleration of the most energetic ions, we used particle tracking in particle-in-cell simulations energy ions originate from a small region of the depth below 1 mu m and the width about the laser focal spot size (3 4 mu m) in target (with gradually increasing density up to the maximum density from the front side) and of a thin foil. On the other hand, t exceeds 5 mu m for the expanded target. When the laser pulse propagates through near-critical density targets, a high density e travels with the laser pulse behind the target. Behind this electron bunch, a relatively long longitudinal electric field is generate ions. Longitudinal electric field can be also generated due to expanding transverse magnetic field, which is observed for the exp

Accession Number: WOS:000502118100002

Conference Title: Conference on Laser Acceleration of Electrons, Protons, and Ions V

Conference Date: APR 01-03, 2019

Conference Location: Prague, CZECH REPUBLIC

Conference Sponsors: SPIE

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Matys, Martin		0000-0002-6215-4246

ISSN: 0277-786X

eISSN: 1996-756X

ISBN: 978-1-5106-2741-3

Record 200 of 235

Title: Human stress detection from the speech in danger situation

Author(s): Partila, P (Partila, Pavol); Tovarek, J (Tovarek, Jaromir); Rozhon, J (Rozhon, Jan); Jalowiczor, J (Jalowiczor, Jakub)

Edited by: Agaian SS; Asari VK; DelMarco SP

Source: MOBILE MULTIMEDIA/IMAGE PROCESSING, SECURITY, AND APPLICATIONS 2019 **Book Series:** Proceedings of SPIE **Volu** UNSP 109930U **DOI:** 10.1117/12.2521405 **Published:** 2019

Abstract: Besides facial expression or gestures, human speech is still the main channel of communication in ordinary human lif content, this signal also contains additional source / human status information. Gender, age, but also the emotional state of ma spoken speech. This research is focused on the classification of the emotional state of man, the stress in particular. Accordingly, database of emergency phone calls. The database contains recordings of the Integrated Rescue System (IRS) of 112 emergency was designed to detect the stress from the human voice. Due to the detection of stress from a neutral (resting) state, the databa speech and human speech in stress. The neutral subgroup consists of voice recordings of the IRS operator. The stress subgroup danger. We have deliberately selected events with great stressful stimuli such as car accident, domestic violence, situations clos speech signal is then pre-processed and analyzed for the feature extraction. The feature vectors represents classifier input data methods such as Support Vector Machine (SVM) or k-Nearest Neighbors (k-NN) classifiers and new artificial intelligence method Neural Networks (CNN) are used to detect and recognize human stress. The applications of achieved results are broad: from ph Health to security components analysis.

Accession Number: WOS:000502067500019

Conference Title: Conference on Mobile Multimedia/Image Processing, Security, and Applications

Conference Date: APR 15, 2019

Conference Location: Baltimore, MD

Conference Sponsors: SPIE

ISSN: 0277-786X

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ISBN: 978-1-5106-2652-2

Close

Close

Web of Science
Page 5 (Records 201 -- 235)
[1 | 2 | 3 | 4 | 5]

Record 201 of 235

Title: Identification of Artifacts and Interesting Celestial Objects in the LAMOST Spectral Survey

Author(s): Skoda, P (Skoda, Petr); Shakurova, K (Shakurova, Ksenia); Koza, J (Koza, Jakub); Palicka, A (Palicka, Andrej)

Edited by: Molinaro M; Shortridge K; Pasian F

Source: ASTRONOMICAL DATA ANALYSIS SOFTWARE AND SYSTEMS XXVI **Book Series:** Astronomical Society of the Pacific Confe 521 **Pages:** 402-405 **Published:** 2019

Abstract: The LAMOST DR1 survey contains about two million spectra labelled by its pipeline as stellar objects of common spec however, a lot of spectra corrupted in some way by both instrumental and processing artifacts, which may mimic spectral prope objects, namely emission lines of Be stars and quasars.
We have tested several clustering methods as well as outlier analysis on a sample of one hundred thousand spectra using Spark cluster consisting of twenty-four sixteen-core nodes. This experiment was motivated by an attempt to find rare objects with inte most dissimilar from all common spectra.
The result of this time-consuming procedure is a list of several hundred candidates where different artifacts are prominent, but emission-line spectra requiring further detailed examination. Many of them may be quasars or even blazars as well as yet unkn mentioning that most of the work benefitted considerably from technologies of the Virtual Observatory.

Accession Number: WOS:000495812900097

Conference Title: 26th Annual Conference for Astronomical Data Analysis Software and Systems (ADASS XXVI)

Conference Date: OCT 16-20, 2016

Conference Location: Italian Natl Inst Astrophys, Trieste Astron Observ, Trieste, ITALY

Conference Sponsors: INAF, ADASS partners, Fondazione CRTrieste, Conserzio Fisica Trieste, SISSA, Altec, E4 Computer Engn, E Trieste, Regione Autonoma Friuli Venezia Giulia, MHPC

Conference Host: Italian Natl Inst Astrophys, Trieste Astron Observ

ISSN: 1050-3390

ISBN: 978-1-58381-929-6

Record 202 of 235

Title: Video Sequence Boundary Labeling with Temporal Coherence

Author(s): Bobak, P (Bobak, Petr); Cmolik, L (Cmolik, Ladislav); Cadik, M (Cadik, Martin)

Edited by: Gavrilova M; Chang J; Thalmann NM; Hitzer E; Ishikawa H

Source: ADVANCES IN COMPUTER GRAPHICS, CGI 2019 **Book Series:** Lecture Notes in Computer Science **Volume:** 11542 **Pages** 10.1007/978-3-030-22514-8_4 **Published:** 2019

Abstract: We propose a method for video sequence boundary labeling which maintains the temporal coherence. The method is the movement of the label boxes only to the horizontal direction, and reserve free space for the movement of the label boxes in proposed method is able to position label boxes in video sequence on a lower number of rows than existing methods, while at t the movement of label boxes. We conducted an extensive user experiment where the proposed method was ranked the best for labeling compared to three existing methods.

Accession Number: WOS:000495360100004

Conference Title: 36th Computer Graphics International Conference (CGI)

Conference Date: JUN 17-20, 2019

Conference Location: Calgary, CANADA

Conference Sponsors: Biometric Technologies Lab, Univ Calgary, VPR Off, Fac Sci, Comp Sci Dept, Alberta Ingenu, CGS

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Bobak, Petr		0000-0003-1914-4592

ISSN: 0302-9743

eISSN: 1611-3349

ISBN: 978-3-030-22514-8; 978-3-030-22513-1

Record 203 of 235

Title: 3-D NLTE Monte Carlo Radiative Transfer Code for Stellar Wind Modeling

Author(s): Fisak, J (Fisak, Jakub); Kubat, J (Kubat, Jiri); Kubatova, B (Kubatova, Brankica); Kromer, M (Kromer, Markus); Krticka,
Edited by: Werner K; Stehle C; Rauch T; Lanz TM
Source: RADIATIVE SIGNATURES FROM THE COSMOS **Book Series:** Astronomical Society of the Pacific Conference Series **Volun** 15-20 **Published:** 2019
Abstract: We present the current state of our 3-D Monte Carlo radiative transfer code for modelling the stellar wind of hot stars. indivisible energy packets proposed by Leon Lucy. Currently the code calculates the emergent spectrum of an input stellar winc developed to solve the NLTE line formation problem in a 3-D model of a stellar wind.
Accession Number: WOS:000494866300003
Conference Title: Conference on Radiative Signatures from the Cosmos
Conference Date: OCT 23-26, 2018
Conference Location: Sorbonne Univ, Paris, FRANCE
Conference Sponsors: Sorbonne Univ, Labex Plas Par (ANR-11-IDEX-0004-02), Observatpore Cote Azur,, CNRS Programme Natl I Observatoire Paris, Univ Arizona, Astron & Steward Observ, LERMA Lab Paris
Conference Host: Sorbonne Univ
ISSN: 1050-3390
ISBN: 978-1-58381-925-8

Record 204 of 235

Title: First record of the rare freshwater alga Tetrasporopsis fuscescens (Chrysomerophyceae, Ochrophyta) in North America
Author(s): Stancheva, R (Stancheva, Rosalina); Skaloud, P (Skaloud, Pavel); Pusztai, M (Pusztai, Martin); Loflen, CL (Loflen, Chac Robert G.)
Source: FOTTEA **Volume:** 19 **Issue:** 2 **Pages:** 163-174 **DOI:** 10.5507/fot.2019.007 **Published:** 2019
Abstract: This study presents the first record of the ochrophyte alga Tetrasporopsis fuscescens in North America, confirmed wit electron microscopic photomicrographs, cytochemical and molecular phylogenetic analyses. T. fuscescens was recorded rarely of only twelve stream sites: nine locations in Southern California and three in Northern California. More than half of the streams characterized by long dry periods. Tetrasporopsis cells were gold-colored, spherical, with a distinct wall, assembled in the perip gelatinous colonies, which start as tubular or sac-like structures, but later become membranous. The cells have 1-2 parietal chl pyrenoid, and reproduction occurs by longitudinal cell division. Other features of the genus are as follows: cells in the colonies a be smaller autospores with remnant cell walls remaining, the colonial mucilage consists of cylindrical dichotomously branched center of the colony to which attach the peripheral cells, and older cells become filled with large oil droplets. A combined gene nuclear SSU rDNA, plastid rbcL, psaA, psbA and psbC showed that T. fuscescens specimens from Europe and U. S. A. formed a G taxa classified in the class Chrysomerophyceae.
Accession Number: WOS:000493808100006
ISSN: 1802-5439

Record 205 of 235

Title: Key Exchange with PUF in NG-PON2 Networks
Author(s): Horvath, T (Horvath, Tomas); Clupek, V (Clupek, Vlastimil); Munster, P (Munster, Petr); Oujezsky, V (Oujezsky, Vaclav)
Book Group Author(s): IEEE
Source: 2019 42ND INTERNATIONAL CONFERENCE ON TELECOMMUNICATIONS AND SIGNAL PROCESSING (TSP) **Pages:** 118-121
Abstract: As next generation passive optical networks (XG-PONs) are currently being deployed, the usability and future deployn stage 2 (NG-PON2) are being called into question. This work provides an overview of basic parameters used in generation (stage The approved recommendations do not include the complete descriptions of these network parameters, but rather the parame distribution and exchange of keys necessary for NG-PON2 communication. This work also summarizes the current state of affai unclonable function (PUF) based improvement in the key exchange procedure that takes place between optical line terminatio unit (ONU). To implement the new key exchange method, it is necessary to define a new physical layer operations, administrati message that is derived from the existing one.
Accession Number: WOS:000493442800026
Conference Title: 42nd International Conference on Telecommunications and Signal Processing (TSP)
Conference Date: JUL 01-03, 2019
Conference Location: Budapest, HUNGARY
Conference Sponsors: IEEE Reg 8, IEEE Hungary Sect, IEEE Czechoslovakia Sect & SP CAS COM Joint Chapter, Sci Assoc Infocom Dept Telecommunicat, Budapest Univ Technol & Econ, Dept Telecommunicat & Media Informat, Czech Tech Univ Prague, Dept T Univ, Dept Elect & Elect Engn,, Istanbul Tech Univ, Elect & Communicat Engn Dept, Josip Juraj Strossmayer Univ Osijek, Fac Elec Technol, Karadeniz Tech Univ, Dept Elect & Elect Engn, Natl Taiwan Univ Sci & Technol, Dept Elect & Comp Engn, Seikei Univ, Gra

Informat Networking Lab, Slovak Univ Technol Bratislava, Inst Multimedia Informat & Commun Technologies, Escola Univ Polite Tech Univ Sofia, Fac Telecommunicat, Univ Paris 8, UFR MITSIC, Lab Informatique Avancee Saint Denis, Univ Politehnica Buchar & Innovat Proc, Univ Ljubljana, Lab Telecommunicat, Univ Patras, Phys Dept, VSB Tech Univ Ostrava, Dept Telecommunicat, W F Elect Engn

ISBN: 978-1-7281-1864-2

Record 206 of 235

Title: High-speed Data Acquisition and Signal Processing Using Cost Effective ARM plus FPGA Processors

Author(s): Dejdar, P (Dejdar, Petr); Munster, P (Munster, Petr); Horvath, T (Horvath, Tomas)

Book Group Author(s): IEEE

Source: 2019 42ND INTERNATIONAL CONFERENCE ON TELECOMMUNICATIONS AND SIGNAL PROCESSING (TSP) **Pages:** 593-596

Abstract: The paper describes the possibilities of data acquisition and data processing from optical sensing systems. There are and their disadvantages when used for more complex single fiber sensor systems in the paper. It is suitable to use some open so commercially available data acquisition cards are more complex and universal which means they have several different inputs/ dimensions. STEMLab 125-14 (Red Pitaya) appears to be the most suitable solution because offers 2 analog inputs and 2 analog standard data processing systems, this is supposed to be an advantage in preprocessing data using programmable logic. This ca transmitted data and can also speed up processing. Thus, the measurement system will be smaller and cheaper. The device cor therefore pulses might be generated using the same clock which enables synchronization of backscatter signal.

Accession Number: WOS:000493442800129

Conference Title: 42nd International Conference on Telecommunications and Signal Processing (TSP)

Conference Date: JUL 01-03, 2019

Conference Location: Budapest, HUNGARY

Conference Sponsors: IEEE Reg 8, IEEE Hungary Sect, IEEE Czechoslovakia Sect & SP CAS COM Joint Chapter, Sci Assoc Infocom Dept Telecommunicat, Budapest Univ Technol & Econ, Dept Telecommunicat & Media Informat, Czech Tech Univ Prague, Dept T Univ, Dept Elect & Elect Engn,, Istanbul Tech Univ, Elect & Communicat Engn Dept, Josip Juraj Strossmayer Univ Osijek, Fac Elec Technol, Karadeniz Tech Univ, Dept Elect & Elect Engn, Natl Taiwan Univ Sci & Technol, Dept Elect & Comp Engn, Seikei Univ, Gra Informat Networking Lab, Slovak Univ Technol Bratislava, Inst Multimedia Informat & Commun Technologies, Escola Univ Polite Tech Univ Sofia, Fac Telecommunicat, Univ Paris 8, UFR MITSIC, Lab Informatique Avancee Saint Denis, Univ Politehnica Buchar & Innovat Proc, Univ Ljubljana, Lab Telecommunicat, Univ Patras, Phys Dept, VSB Tech Univ Ostrava, Dept Telecommunicat, W F Elect Engn

ISBN: 978-1-7281-1864-2

Record 207 of 235

Title: Polarization Changes as Early Warning System in Optical Fiber Networks

Author(s): Slapak, M (Slapak, Martin); Vojtech, J (Vojtech, Josef); Munster, P (Munster, Petr)

Book Group Author(s): IEEE

Source: 2019 42ND INTERNATIONAL CONFERENCE ON TELECOMMUNICATIONS AND SIGNAL PROCESSING (TSP) **Pages:** 597-600

Abstract: In presented work, we focus on an experimental comparison of high sensitivity and performance interferometric base narrowband laser and methods based on the passive state of polarization changes detection in fiber with simple on-off keying r stress from the environment causes changes in the state of polarization. Therefore it is possible to use its detection as an early v The results show that cheap and simple setup with detection of a change of state of polarization achieves a sufficient sensitivity up to 100 Hz and also the short intensive pulses like from digging.

Accession Number: WOS:000493442800130

Conference Title: 42nd International Conference on Telecommunications and Signal Processing (TSP)

Conference Date: JUL 01-03, 2019

Conference Location: Budapest, HUNGARY

Conference Sponsors: IEEE Reg 8, IEEE Hungary Sect, IEEE Czechoslovakia Sect & SP CAS COM Joint Chapter, Sci Assoc Infocom Dept Telecommunicat, Budapest Univ Technol & Econ, Dept Telecommunicat & Media Informat, Czech Tech Univ Prague, Dept T Univ, Dept Elect & Elect Engn,, Istanbul Tech Univ, Elect & Communicat Engn Dept, Josip Juraj Strossmayer Univ Osijek, Fac Elec Technol, Karadeniz Tech Univ, Dept Elect & Elect Engn, Natl Taiwan Univ Sci & Technol, Dept Elect & Comp Engn, Seikei Univ, Gra Informat Networking Lab, Slovak Univ Technol Bratislava, Inst Multimedia Informat & Commun Technologies, Escola Univ Polite Tech Univ Sofia, Fac Telecommunicat, Univ Paris 8, UFR MITSIC, Lab Informatique Avancee Saint Denis, Univ Politehnica Buchar & Innovat Proc, Univ Ljubljana, Lab Telecommunicat, Univ Patras, Phys Dept, VSB Tech Univ Ostrava, Dept Telecommunicat, W F Elect Engn

ISBN: 978-1-7281-1864-2

Record 208 of 235

Title: European Union Funded Projects for Time and Frequency Transfer in Optical Fiber

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

Book Group Author(s): Inst Navigat

Source: PROCEEDINGS OF THE 50TH ANNUAL PRECISE TIME AND TIME INTERVAL SYSTEMS AND APPLICATIONS MEETING **Book** and Time Interval Systems and Applications Meeting **Pages:** 235-241 **Article Number:** UNSP 16769 **DOI:** 10.33012/2019.16769

Abstract: This paper focuses on past, current and ready-to-start time and frequency metrology projects taking place in Europe a frequency transfer in optical fiber. It addresses both EURAMET and H2020 scope projects. We also briefly describe the involvem Networks (NRENs). As the operation of dedicated optical fiber infrastructure is very expensive, NMIs started to cooperate with N optical data networks and can provide part of the optical spectrum for time and frequency applications.
Horizon 2020 is the European Union framework programme for research and innovation. One of its goals is to reinforce and exte science base and to consolidate the European research area to make the research and innovation system more competitive on a also supports several metrology projects, either directly or in cooperation with the association EURAMET. Horizon 2020, as the b Innovation programme is scheduled for 7 years (2014 to 2020) and has budget of 80 billion (sic) for projects funding.

Accession Number: WOS:000492297800019

Conference Title: 50th Annual Precise Time and Time Interval Systems and Applications Meeting

Conference Date: JAN 28-31, 2019

Conference Location: Reston, VA

Conference Sponsors: Inst Navigat

ISSN: 2333-2085

ISBN: 978-0-936406-20-6

Record 209 of 235

Title: English Dataset For Automatic Forum Extraction

Author(s): Sido, J (Sido, Jakub); Konopik, M (Konopik, Miloslav); Prazak, O (Prazak, Ondrej)

Source: COMPUTACION Y SISTEMAS **Volume:** 23 **Issue:** 3 **Pages:** 765-771 **DOI:** 10.13053/CyS-23-3-3259 **Published:** 2019

Abstract: This paper describes the process of collecting, maintaining and exploiting an English dataset of web discussions. The discussions with hand-annotated posts in the context of a tree structure of a web page. Each post consists of username, date, te author. The dataset contains 79 different websites with at least 500 pages from each. Each web page consists of a tree structure from selected web pages. In the paper, we also describe algorithms trained on the dataset. The algorithms employ basic archite words with an SVM classifier and an LSTM network) to set a baseline for the dataset.

Accession Number: WOS:000489136900014

ISSN: 1405-5546

eISSN: 2007-9737

Record 210 of 235

Title: Enriching Word Embeddings with Global Information and Testing on Highly Inflected Language

Author(s): Svoboda, L (Svoboda, Lukas); Brychcin, T (Brychcin, Tomas)

Source: COMPUTACION Y SISTEMAS **Volume:** 23 **Issue:** 3 **Pages:** 773-783 **DOI:** 10.13053/CyS-23-3-3268 **Published:** 2019

Abstract: In this paper we evaluate our new approach based on the Continuous Bag-of-Words and Skip-gram models enriched v information on highly inflected Czech language and compare it with English results. As a source of information we use Wikipedi organized in a hierarchy of categories. These categories provide useful topical information about each article. Both models are similarity and word analogy datasets. Proposed models outperform other word representation methods when similar size of tra provide similar performance especially with methods trained on much larger datasets.

Accession Number: WOS:000489136900015

ISSN: 1405-5546

eISSN: 2007-9737

Record 211 of 235

Title: The molecular and morphometric identification of Dictyocaulus capreolus in clinically affected roe deer (Capreolus capre

Author(s): Jurankova, J (Jurankova, Jana); Jirsova, D (Jirsova, Dagmar); Pafco, B (Pafco, Barbora); Forejtek, P (Forejtek, Pavel)

Source: VETERINARNI MEDICINA **Volume:** 64 **Issue:** 9 **Pages:** 386-391 **DOI:** 10.17221/9/2019-VETMED **Published:** 2019

Abstract: The poor state of health and increased mortality rate of young roe deer, as reported by South Moravian hunters, cause of adult nematodes in the lungs of roe deer prompted us to identify the parasites using a combination of morphological measu SSU rRNA analysis. The study was conducted in a 294 ha game reserve in South Moravia, Czech Republic. Molecular and morph

to identify adult nematodes collected from the respiratory tracts of nine 4-5 months old roe deer in poor health (low body weigl quality, and, in some cases, symptoms of diarrhoea). The morphological identification was based on a combination of adult wo corresponding to Dictyocaulus capreolus. A small subunit rRNA (SSU) partial sequence analysis showed the highest identity scc the sequences of D. capreolus from a roe deer (GenBank: AY168859) from Sweden and the outcomes of the phylogenetic analys high branch support for two groups, with our sequences forming a well-supported clade with D. capreolus and Dictyocaulus sp. (FJ589016) and Dictyocaulus sp. ex Rupicapra rupicapra (FJ589019) sequences from Spain. The examined roe deer have shown s anorexia, and respiratory tract inflammation indicating that there might be a connection to the clinical importance of the Dicty

Accession Number: WOS:000488083000002

ISSN: 0375-8427

eISSN: 1805-9392

Record 212 of 235

Title: Improving Domain-Independent Planning via Critical Section Macro-Operators

Author(s): Chrpa, L (Chrpa, Lukas); Vallati, M (Vallati, Mauro)

Book Group Author(s): AAAI

Source: THIRTY-THIRD AAAI CONFERENCE ON ARTIFICIAL INTELLIGENCE / THIRTY-FIRST INNOVATIVE APPLICATIONS OF ARTIFIC CONFERENCE / NINTH AAAI SYMPOSIUM ON EDUCATIONAL ADVANCES IN ARTIFICIAL INTELLIGENCE **Pages:** 7546-7553 **Publish**

Abstract: Macro-operators, macros for short, are a well-known technique for enhancing performance of planning engines by pr state space. Existing macro learning systems usually generate macros from most frequent sequences of actions in training plans frequently used sequences of actions over meaningful activities to be performed for solving planning tasks.

This paper presents a technique that, inspired by resource locking in critical sections in parallel computing, learns macros capt limited resource (e.g., a robotic hand) is used. In particular, such macros capture the whole activity in which the resource is "loc holding an object) and thus "bridge" states in which the resource is locked and cannot be used. We also introduce an "aggressiv that removes original operators superseded by macros from the domain model. Usefulness of macros is evaluated on several st wide range of benchmarks from the learning tracks of the 2008 and 2011 editions of the International Planning Competition.

Accession Number: WOS:000486572502010

Conference Title: 33rd AAAI Conference on Artificial Intelligence / 31st Innovative Applications of Artificial Intelligence Conferen Educational Advances in Artificial Intelligence

Conference Date: JAN 27-FEB 01, 2019

Conference Location: Honolulu, HI

Conference Sponsors: Assoc Advancement Artificial Intelligence

ISBN: 978-1-57735-809-1

Record 213 of 235

Title: Operator Mutexes and Symmetries for Simplifying Planning Tasks

Author(s): Fiser, D (Fiser, Daniel); Torralba, A (Torralba, Alvaro); Shleyfman, A (Shleyfman, Alexander)

Book Group Author(s): AAAI

Source: THIRTY-THIRD AAAI CONFERENCE ON ARTIFICIAL INTELLIGENCE / THIRTY-FIRST INNOVATIVE APPLICATIONS OF ARTIFIC CONFERENCE / NINTH AAAI SYMPOSIUM ON EDUCATIONAL ADVANCES IN ARTIFICIAL INTELLIGENCE **Pages:** 7586-7593 **Publish**

Abstract: Simplifying classical planning tasks by removing operators while preserving at least one optimal solution can signific performance of planners. In this paper, we introduce the notion of operator mutex, which is a set of operators that cannot all be optimal plan. We propose four different methods for inference of operator mutexes and experimentally verify that they can be f planning tasks. We show how operator mutexes can be used in combination with structural symmetries to safely remove opera

Accession Number: WOS:000486572502015

Conference Title: 33rd AAAI Conference on Artificial Intelligence / 31st Innovative Applications of Artificial Intelligence Conferen Educational Advances in Artificial Intelligence

Conference Date: JAN 27-FEB 01, 2019

Conference Location: Honolulu, HI

Conference Sponsors: Assoc Advancement Artificial Intelligence

ISBN: 978-1-57735-809-1

Record 214 of 235

Title: DIC IMAGE SEGMENTATION OF DENSE CELL POPULATIONS BY COMBINING DEEP LEARNING AND WATERSHED

Author(s): Lux, F (Lux, Flip); Matula, P (Matula, Petr)

Book Group Author(s): IEEE

Source: 2019 IEEE 16TH INTERNATIONAL SYMPOSIUM ON BIOMEDICAL IMAGING (ISBI 2019) **Book Series:** IEEE International Syr Imaging **Pages:** 236-239 **Published:** 2019

Abstract: Image segmentation of dense cell populations acquired using label-free optical microscopy techniques is a challengir propose a novel approach based on a combination of deep learning and the watershed transform to segment differential interf with high accuracy. The main idea of our approach is to train a convolutional neural network to detect both cellular markers an these predictions, to split the individual cells using the watershed transform. The approach was developed based on the image populations included in the Cell Tracking Challenge database, Our approach was ranked the best in terms of segmentation, det performance as evaluated on the challenge datasets.

Accession Number: WOS:000485040000055

Conference Title: 16th IEEE International Symposium on Biomedical Imaging (ISBI)

Conference Date: APR 08-11, 2019

Conference Location: Venice, ITALY

Conference Sponsors: Inst Elect & Elect Engineers, IEEE Engn Med & Biol Soc, IEEE Signal Proc Soc, Canon Med Res Europe Ltd, Intelligence, Baidu, GSK, Kitware

ISSN: 1945-7928

ISBN: 978-1-5386-3641-1

Record 215 of 235

Title: USING EXTREME GRADIENT BOOSTING TO DETECT GLOTTAL CLOSURE INSTANTS IN SPEECH SIGNAL

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

Book Group Author(s): IEEE

Source: 2019 IEEE INTERNATIONAL CONFERENCE ON ACOUSTICS, SPEECH AND SIGNAL PROCESSING (ICASSP) **Book Series:** Int Acoustics Speech and Signal Processing ICASSP **Pages:** 6515-6519 **Published:** 2019

Abstract: In this paper, we continue to investigate the use of classifiers for the automatic detection of glottal closure instants (G We focus on extreme gradient boosting (XGB), a fast and powerful implementation of a gradient boosting algorithm. We show tl classifiers, achieving GCI detection accuracy F1 = 98:55% and AUC = 99:90%. The proposed XGB model is also shown to outperfc detection algorithms on publicly available databases. Despite using much less training data, the performance of XGB is compar neural network based approach, especially when it is tested on voices that were not included in the training data.

Accession Number: WOS:000482554006149

Conference Title: 44th IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)

Conference Date: MAY 12-17, 2019

Conference Location: Brighton, ENGLAND

Conference Sponsors: Inst Elect & Elect Engineers, Inst Elect & Elect Engineers Signal Proc Soc

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Tihelka, Daniel	AAD-1622-2019	

ISSN: 1520-6149

ISBN: 978-1-4799-8131-1

Record 216 of 235

Title: Detection of changes in the qualitative parameters for LoRaWAN and SigFox network

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

Edited by: Blowers M; Hall RD; Dasari VR

Source: DISRUPTIVE TECHNOLOGIES IN INFORMATION SCIENCES II **Book Series:** Proceedings of SPIE **Volume:** 11013 **Article N** 10.1117/12.2518853 **Published:** 2019

Abstract: It is estimated, that the number of connected Internet of Things (IoT) devices around the world could increase dramat ranging from 25 billion to 50 billion devices in 2025. As the IoT area is wider and wider and the number of connected IoT devices appears that the issue of security is more up to date. The paper deals with LoRaWAN and Sigfox networks belonging to the LPW Network) category, where we focus on detection of the end device movement in a network based on the qualitative parameters this work is a software solution to notice the owner of the end device about the location change. As a testbed, we use LoRaWAN infrastructure covering the area of Czech Republic. For Sigfox solution we use the public network provided by SimpleCell compa actual parameters with which base station received messages. Detection serves as a measure against an attacker performing a physical movement of a statically-located end device activated by authentication methods. Based on the experimental simulati we have summed up the attack into individual points, according to which we subsequently constructed a countermeasure prin

This principle was applied to an algorithm that could be integrated into the gateway in case of LoRaWAN network and impleme Sigfox solution.

Accession Number: WOS:000484762100019

Conference Title: Conference on SPIE Disruptive Technologies in Information Sciences II

Conference Date: APR 15-16, 2019

Conference Location: Baltimore, MD

Conference Sponsors: SPIE

Author Identifiers:

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Safarik, Jakub		0000-0002-3360-2302

ISSN: 0277-786X

eISSN: 1996-756X

ISBN: 978-1-5106-2692-8

Record 217 of 235

Title: Classification with Costly Features Using Deep Reinforcement Learning

Author(s): Janisch, J (Janisch, Jaromir); Pevny, T (Pevny, Tomas); Lisy, V (Lisy, Viliam)

Book Group Author(s): AAAI

Source: THIRTY-THIRD AAAI CONFERENCE ON ARTIFICIAL INTELLIGENCE / THIRTY-FIRST INNOVATIVE APPLICATIONS OF ARTIFIC CONFERENCE / NINTH AAAI SYMPOSIUM ON EDUCATIONAL ADVANCES IN ARTIFICIAL INTELLIGENCE **Pages:** 3959-3966 **Publish**

Abstract: We study a classification problem where each feature can be acquired for a cost and the goal is to optimize a trade-off classification error and the feature cost. We revisit a former approach that has framed the problem as a sequential decision-ma Q-learning with a linear approximation, where individual actions are either requests for feature values or terminate the episode decision. On a set of eight problems, we demonstrate that by replacing the linear approximation with neural networks the appr the state-of-the-art algorithms developed specifically for this problem. The approach is flexible, as it can be improved with any enhancement, it allows inclusion of pre-trained high-performance classifier, and unlike prior art, its performance is robust acro

Accession Number: WOS:000485292603120

Conference Title: 33rd AAAI Conference on Artificial Intelligence / 31st Innovative Applications of Artificial Intelligence Conferen Educational Advances in Artificial Intelligence

Conference Date: JAN 27-FEB 01, 2019

Conference Location: Honolulu, HI

Conference Sponsors: Assoc Advancement Artificial Intelligence

ISBN: 978-1-57735-809-1

Record 218 of 235

Title: AMINO-SUBSTITUTED NAPHTHALENE SULFONIC ACID/GRAPHENE COMPOSITE AS METAL -FREE CATALYSTS FOR OXYGEN F

Author(s): Getachew, T (Getachew, Teklewold); Addis, F (Addis, Fitsum); Beyene, T (Beyene, Taye); Mehretie, S (Mehretie, Solom Shimelis)

Source: BULLETIN OF THE CHEMICAL SOCIETY OF ETHIOPIA **Volume:** 33 **Issue:** 2 **Pages:** 359-372 **DOI:** 10.4314/bcse.v33i2.16 **F**

Abstract: Composites of reduced graphene oxide (rGO) and conducting polymers synthesized from 8-amino-2-naphthalene sul 1-naphthalene sulfonic acid (5-ANSA), 2-amino-1-naphthalene sulfonic acid (2-ANSA), and 4-amino-l-naphthalene sulfonic (4-A an electrocatalyst in oxygen reduction reaction (ORR). The electrocatalytic activities were examined in oxygen saturated 0.1 M K linear sweep voltammetry. The best performing polymer composite was found to be GC/poly(8-ANSA)/rGO, with an enhanced e the rGO only and poly(8-ANSA) only films. More than 100 mV positive shift in the onset potential and 1.6 times increase in curren catalytic activity of 2-ANSA, 4-ANSA, 5-ANSA, and 8-ANSA was also validated by density functional theory (DFT). Our calculation catalytic activity for 8-ANSA than that of 2-ANSA, 4-ANSA, and 5-ANSA.

Accession Number: WOS:000482782000016

Author Identifiers:

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Admassie, Shimelis		0000-0001-9484-0972

ISSN: 1011-3924

eISSN: 1726-801X

Record 219 of 235

Title: EFFECT OF A REALISTIC THREE-BODY FORCE ON THE ENERGY SPECTRA OF C-13(Lambda), O-17(Lambda), K-40(Lambda) A

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

Source: ACTA PHYSICA POLONICA B PROCEEDINGS SUPPLEMENT **Volume:** 12 **Issue:** 3 **Pages:** 657-664 **DOI:** 10.5506/APhysPolE 2019

Abstract: We adopt the Hartree-Fock (HF) method and the nucleon-Lambda Tamm-Dancoff Approximation (N Lambda TDA) to s selected medium mass hypernuclei composed of a Lambda hyperon bound to an even-even and odd-even nuclear cores. Our c using the Y N LO potential plus the chiral potential NNLOsat, which includes explicitly the 3-body NNN force. This component, w of the nuclear cores and the relative distances between levels or group of levels of the hypernuclear spectra, strongly reduces th that the inclusion of more complex configurations is badly needed.

Accession Number: WOS:000481533000019

Conference Title: 25th Nuclear Physics Workshop on Structure and Dynamics of Atomic Nuclei

Conference Date: SEP 25-30, 2018

Conference Location: Kazimierz Dolny, POLAND

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
De Gregorio, Giovanni	AAH-2437-2019	0000-0003-0253-915X
Knapp, Frantisek	P-1429-2017	0000-0002-7708-6290

ISSN: 1899-2358

eISSN: 2082-7865

Record 220 of 235

Title: Monte Carlo Continual Resolving for Online Strategy Computation in Imperfect Information Games

Author(s): Sustr, M (Sustr, Michal); Kovarik, V (Kovarik, Vojtech); Lisy, V (Lisy, Viliam)

Book Group Author(s): Assoc Comp Machinery

Source: AAMAS '19: PROCEEDINGS OF THE 18TH INTERNATIONAL CONFERENCE ON AUTONOMOUS AGENTS AND MULTIAGENT S 224-232 **Published:** 2019

Abstract: Online game playing algorithms produce high quality strategies with a fraction of memory and computation required Continual Resolving (CR) is a recent theoretically sound approach to online game playing that has been used to outperform hur However, parts of the algorithm were specific to poker, which enjoys many properties not shared by other imperfect informatio domain independent formulation of CR applicable to any twoplayer zero sum extensive form games (EFGs). It works with an ab which can be instantiated by various EFG solvers. We further describe and implement its Monte Carlo variant (MCCR) which use Regret Minimization (MCCFR) as a resolver. We prove the correctness of CR and show an O(T-1/2) dependence of MCCR's exploit time. Furthermore, we present an empirical comparison of MCCR with incremental tree building to Online Outcome Sampling a several domains.

Accession Number: WOS:000474345000030

Conference Title: 18th International Conference on Autonomous Agents and MultiAgent Systems (AAMAS)

Conference Date: MAY 13-17, 2019

Conference Location: Montreal, CANADA

Conference Sponsors: Assoc Comp Machinery, Int Fdn Autonomous Agents & MultiAgent Syst, NSF, Artificial Intelligence Journa Morgan, DeepMind, ACM SIGAI, Concordia Univ

ISBN: 978-1-4503-6309-9

Record 221 of 235

Title: GENETIC ALGORITHM FOR THE CONTINUOUS LOCATION-ROUTING PROBLEM

Author(s): Rybickova, A (Rybickova, A.); Mockova, D (Mockova, D.); Teichmann, D (Teichmann, D.)

Source: NEURAL NETWORK WORLD **Volume:** 29 **Issue:** 3 **Pages:** 173-187 **DOI:** 10.14311/NNW.2019.29.012 **Published:** 2019

Abstract: This paper focuses on the continuous location-routing problem that comprises of the location of multiple depots fron determining the routes of vehicles assigned to these depots. The objective of the problem is to design the delivery system of de total cost is minimal. The standard location-routing problem considers a finite number of possible locations. The continuous lo allows location to infinite number of locations in a given region and makes the problem much more complex. We present a gen both location and routing subproblems simultaneously.

Accession Number: WOS:000475843600004

ISSN: 1210-0552

Record 222 of 235

Title: Design of a High-Throughput Match Search Unit for Lossless Compression Algorithms

Author(s): Bartik, M (Bartik, Matej); Benes, T (Benes, Tomas); Kubalik, P (Kubalik, Pavel)

Edited by: Chakrabarti S; Saha HN

Source: 2019 IEEE 9TH ANNUAL COMPUTING AND COMMUNICATION WORKSHOP AND CONFERENCE (CCWC) **Pages:** 732-738 **Pu**

Abstract: This paper presents an attempt to combine recent research in fields of hardware-and software-based high-throughpu compression algorithms and their implementations, resulting into a case study focusing on one of the most critical parts of com Search Unit (MSU) and its parallelization. The presented FPGA design combines ideas of the LZ4 algorithm (which is derived fro with the state of the art hardware architectures for lossless compression also based on LZ77. This approach might lead to a sma efficient "building block" for modern implementations of hardware driven lossless compression algorithms. The presented des the main problem of the LZ77 family, namely the construction of and searching in a compression dictionary. Particularly, we co with multi-ported memory in order to improve the bandwidth of the dictionary and the Fibonacci hashing principle originating decrease latency of the MSU and to achieve overall higher throughput rate. For the design synthesis an FPGA of the Xilinx Virtex

Accession Number: WOS:000469462800120

Conference Title: 9th IEEE Annual Computing and Communication Workshop and Conference (CCWC)

Conference Date: JAN 07-09, 2019

Conference Location: Univ Nevada, Las Vegas, NV

Conference Sponsors: IEEE, UNLV, IEEE Reg R1, IEEE Reg 6, IEEE USA, Inst Engn & Management, Univ Engn & Management

Conference Host: Univ Nevada

ISBN: 978-1-7281-0554-3

Record 223 of 235

Title: Ultra High Resolution Jitter Measurement Method for Ethernet Based Networks

Author(s): Hynek, K (Hynek, Karel); Benes, T (Benes, Tomas); Bartik, M (Bartik, Matej); Kubalik, P (Kubalik, Pavel)

Edited by: Chakrabarti S; Saha HN

Source: 2019 IEEE 9TH ANNUAL COMPUTING AND COMMUNICATION WORKSHOP AND CONFERENCE (CCWC) **Pages:** 847-851 **Pu**

Abstract: This document presents a new approach to network jitter measurement and analysis in asynchronous data networks developed monitoring device is capable to analyze an incoming stream speed of 1 Gb/s with the resolution up to 8 ns. The syste speeds up to 100 Gb/s networks. The presented architecture can provide several statistical functions such as measuring a netw Histograms method providing the mean value and peak-to-peak value as well. The architecture was implemented and tested or chip using Avnet AES-KU040-DB-G development board.

Accession Number: WOS:000469462800138

Conference Title: 9th IEEE Annual Computing and Communication Workshop and Conference (CCWC)

Conference Date: JAN 07-09, 2019

Conference Location: Univ Nevada, Las Vegas, NV

Conference Sponsors: IEEE, UNLV, IEEE Reg R1, IEEE Reg 6, IEEE USA, Inst Engn & Management, Univ Engn & Management

Conference Host: Univ Nevada

ISBN: 978-1-7281-0554-3

Record 224 of 235

Title: DNA methylation and hydroxymethylation patterns in acute myeloid leukemia patients with mutations in DNMT3A and ID

Author(s): Sestakova, S (Sestakova, Sarka); Krejcik, Z (Krejcik, Zdenek); Folta, A (Folta, Adam); Cerovska, E (Cerovska, Ela); Salek MD (Merkerova, Michaela Dostalova); Pecherkova, P (Pecherkova, Pavla); Racil, Z (Racil, Zdenek); Mayer, J (Mayer, Jiri); Cetkovsk Remasova, H (Remasova, Hana)

Source: CANCER BIOMARKERS **Volume:** 25 **Issue:** 1 **Pages:** 43-51 **DOI:** 10.3233/CBM-182176 **Published:** 2019

Abstract: BACKGROUND: Aberrant epigenetic patterns are a hallmark of acute myeloid leukemia (AML). Mutations in profound e and IDH1/2 often occur concurrently in AML.

OBJECTIVES: The aim was to analyze DNA methylation, hydroxymethylation and mRNA expression profiles in AML with mutatio (individually and in combinations).

METHODS: Infinium MethylationEPIC BeadChip (Illumina) covering 850,000 CpGs was utilized. The validation of hydroxy-/methy pyrosequencing. HumanHT-12 v4 Expression BeadChip (Illumina) was used for expression examination.

RESULTS: Hierarchical clustering analysis of DNA hydroxy-/methylation data revealed clusters corresponding to DNMT3A and ID healthy controls. Samples with concurrent presence of DNMT3A and IDH1/2 mutations displayed mixed DNA hydroxy-/methylat clustering to healthy controls. Numbers and levels of DNA hydroxymethylation were low. Uniformly hypermethylated loci in AM mutations were enriched for immune response and apoptosis related genes, among which hypermethylation of granzyme B (G

associated with inferior overall survival of AML patients (P = 0.035).
CONCLUSIONS: Distinct molecular background results in specific DNA hydroxy-/methylation profiles in AML. Site-specific DNA h
are much less frequent in AML pathogenesis compared to DNA methylation. Methylation levels of enhancer located upstream G
AML prognostication models.

Accession Number: WOS:000469000100005

PubMed ID: 30988238

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Remesova, Hana	G-3708-2017	0000-0002-2967-8355

ISSN: 1574-0153

eISSN: 1875-8592

Record 225 of 235

Title: UNBIASED ESTIMATION OF NORWAY SPRUCE (PICEA ABIES L. KARST.) CHLOROPLAST STRUCTURE: HETEROGENEITY WITH
UNDER DIFFERENT IRRADIANCE AND [CO2]

Author(s): Kubinova, Z (Kubinova, Zuzana); Glanc, N (Glanc, Natalia); Radochova, B (Radochova, Barbora); Lhotakova, Z (Lhotak
(Janacek, Jiri); Kubinova, L (Kubinova, Lucie); Albrechtova, J (Albrechtova, Jana)

Source: IMAGE ANALYSIS & STEREOLOGY **Volume:** 38 **Issue:** 1 **Pages:** 83-94 **DOI:** 10.5566/ias.2005 **Published:** 2019

Abstract: The main objective of this study was to find out whether the selected chloroplast characteristics measured in the mes
needle surface (i.e., the first mesophyll layer) could be representative for the whole needle cross section. Two chloroplast samp
on Norway spruce needles during the investigation of the effects of different levels of air CO2 concentration and irradiance: (i) s
mesophyll layer, and (ii) systematic uniform random (SUR) sampling. The selected characteristics were: (i) chloroplast area, (ii)
starch areal density on median chloroplast cross sections, and (iv) chloroplast number per unit of needle volume. It was shown
was not representative for estimating all evaluated characteristics except the chloroplast area. Sampling only there caused obta
while SUR sampling gave unbiased estimations at the cost of longer measuring time. The major effect of studied factors was in
starch grain area, which were larger in sun needles in elevated CO2 concentration in comparison with sun needles in ambient C
conclusion, it was demonstrated that the first layer of mesophyll is not always representative for the needle cross section. If tec
recommended for analysis of chloroplast ultrastructure. The simplified sampling design can be applied, e.g., for comparisons o
However, it should be combined with other approaches to characterize the chloroplast function and the results carefully consid

Accession Number: WOS:000464195100009

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Janacek, Jiri	B-7932-2012	
Kubinova, Lucie	B-6803-2012	
Radochova, Barbora	B-8935-2012	0000-0002-5869-539X
Albrechtova, Jana		0000-0001-6912-1992

ISSN: 1580-3139

Record 226 of 235

Title: Cross-platform Data Analysis Reveals a Generic Gene Expression Signature for Microsatellite Instability in Colorectal Canc

Author(s): Pacinkova, A (Pacinkova, Anna); Popovici, V (Popovici, Vlad)

Source: BIOMED RESEARCH INTERNATIONAL **Article Number:** 6763596 **DOI:** 10.1155/2019/6763596 **Published:** 2019

Abstract: The dysfunction of the DNA mismatch repair system results in microsatellite instability (MSI). MSI plays a central role i
multiple human cancers. In colon cancer, despite being associated with resistance to 5-fluorouracil treatment, MSI is a favourab
gastric and endometrial cancers, its prognostic value is not so well established. Nevertheless, recognising the MSI tumours may
the therapeutic effect of immune checkpoint inhibitors. Several gene expression signatures were trained on microarray data se
regulatory mechanisms underlying microsatellite instability in colorectal cancer. A wealth of expression data already exists in th
sets. However, the RNA-seq has become a routine for transcriptome analysis. A new MSI gene expression signature presented h
across two different platforms, microarrays and RNA-seq. In the case of colon cancer, its estimated performance was (i) AUC = 0.
RNA-seq and (ii) AUC = 0.95, 95% CI = (0.92 - 0.97) on microarray. The 25-gene expression signature was also validated in two inc
cancer data sets. Despite being derived from colorectal cancer, the signature maintained good performance on RNA-seq and mi
sets (AUC = 0.90, 95% CI = (0.85 - 0.94) and AUC = 0.83, 95% CI = (0.69 - 0.97), respectively). Furthermore, this classifier retained h
classifying RNA-seq endometrial cancers (AUC = 0.71, 95% CI = (0.62 - 0.81). These results indicate that the new signature was ab
specific differences while preserving the underlying biological differences between MSI/MSS phenotypes in colon cancer sampl

Accession Number: WOS:000463063900001
PubMed ID: 31008109
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Popovici, Vlad C.	C-2039-2008	0000-0002-1311-9188

ISSN: 2314-6133
eISSN: 2314-6141

Record 227 of 235
Title: Learning to predict soccer results from relational data with gradient boosted trees
Author(s): Hubacek, O (Hubacek, Ondrej); Sourek, G (Sourek, Gustav); Zelezny, F (Zelezny, Filip)
Source: MACHINE LEARNING **Volume:** 108 **Issue:** 1 **Pages:** 29-47 **DOI:** 10.1007/s10994-018-5704-6 **Published:** JAN 2019
Abstract: We describe our winning solution to the 2017's Soccer Prediction Challenge organized in conjunction with the MLJ's s
Learning for Soccer. The goal of the challenge was to predict outcomes of future matches within a selected time-frame from diff
A dataset of over 200,000 past match outcomes was provided to the contestants. We experimented with both relational and fea
predictive models from the provided data. We employed relevant latent variables computable from the data, namely so called p
based on the PageRank method. A method based on manually constructed features and the gradient boosted tree algorithm pe
validation set and the challenge test set. We also discuss the validity of the assumption that probability predictions on the three
should be monotone, underlying the RPS measure of prediction quality.
Accession Number: WOS:000458551700003
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Hubacek, Ondrej		0000-0003-4449-0083

ISSN: 0885-6125
eISSN: 1573-0565

Record 228 of 235
Title: Data-driven activity scheduler for agent-based mobility models
Author(s): Drchal, J (Drchal, Jan); Certicky, M (Certicky, Michal); Jakob, M (Jakob, Michal)
Source: TRANSPORTATION RESEARCH PART C-EMERGING TECHNOLOGIES **Volume:** 98 **Pages:** 370-390 **DOI:** 10.1016/j.trc.2018.
Abstract: Activity-based modelling is a modern agent-based approach to travel demand modelling, in which the transport dem
agent's needs to perform certain activities at specific places and times. The agent's mobility is considered in a broader context,
based models to produce more realistic trip chains, compared to traditional trip based models. The core of any activity-based n
a software component producing sequences of agent's daily activities interconnected by trips, called activity schedules. Traditi
used to rely heavily on hard-coded knowledge of transport behaviour experts. We introduce the concept of a Data-Driven Activi
replaces numerous expert-designed components and their intricately engineered interactions with a collection of machine lear
is significantly simpler, making it easier to deploy and maintain. This shift towards data-driven, machine learning based approa
increased availability of mobility-related data. We demonstrate DDAS concept using our own proof-of-concept implementation,
and compare the validity of the resulting model to one of the rule-based alternatives using the Validation Framework for Activit
Accession Number: WOS:000457666200022
Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Drchal, Jan		0000-0003-0466-275X

ISSN: 0968-090X

Record 229 of 235
Title: The W UMa binaries USNO-A2.0 1350-17365531, V471 Cas, V479 Lac and V560 Lac: light curve solutions and global parame
Author(s): Kjurkchieva, DP (Kjurkchieva, Diana P.); Popov, VA (Popov, Velimir A.); Eneva, Y (Eneva, Yordanka); Petrov, NI (Petrov,
Source: RESEARCH IN ASTRONOMY AND ASTROPHYSICS **Volume:** 19 **Issue:** 1 **Article Number:** 014 **DOI:** 10.1088/1674-4527/19,
Abstract: We present photometric observations in Sloan filters g', i' of the eclipsing W UMa stars USNO-A2.0 1350-17365531, V47
The sinusoidal-like O - C diagram of V471 Cas indicates the presence of a third body with mass 0.12 M-circle dot (a red dwarf) at
O - C diagram of V479 Lac reveals a period decrease of dP/dt = -1.69 x 10(-6)d yr(-1). The results of the light curve solutions are: (

binaries with small fill-out factors; (ii) their components are F-K stars, comparable in size, whose temperature differences are be partial eclipses and to limit the possible mass ratios we carried out two-step q-search analysis. The target global parameters (lu were obtained on the basis of their Gaia distances and the results of our light curve solutions. The obtained total mass of V560 L than the lower mass limit for presently known W UMa binaries of 1.0 - 1.2 M-circle dot, i.e. this target is a peculiar overcontact sy

Accession Number: WOS:000456345900014

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Popov, Velimir		0000-0003-1415-9525

ISSN: 1674-4527

Record 230 of 235

Title: Estimating sequence similarity from read sets for clustering next-generation sequencing data

Author(s): Rysavy, P (Rysavy, Petr); Zelezny, F (Zelezny, Filip)

Source: DATA MINING AND KNOWLEDGE DISCOVERY **Volume:** 33 **Issue:** 1 **Pages:** 1-23 **DOI:** 10.1007/s10618-018-0584-8 **Publish**

Abstract: Computing mutual similarity of biological sequences such as DNA molecules is essential for significant biological task clustering of genomes. Current sequencing technologies do not provide the content of entire biological sequences; rather they small substrings called reads, sampled at random places of the target sequence. To estimate similarity of two sequences from t one may try to reconstruct each one first from its read set, and then employ conventional (dis)similarity measures such as the e sequences. Due to the nature of data, sequence assembly often cannot provide a single putative sequence that matches the tru instead to estimate the similarities directly from the read sets. Our approach is based on an adaptation of the Monge-Elkan simi databases, avoiding the sequence assembly step. For low-coverage (i.e. small) read set samples, it yields a better approximatio similarities. This in turn results in better clustering in comparison to the first-assemble-then-cluster approach. Put differently, fo our approach requires smaller read sets and thus entails reduced wet-lab costs.

Accession Number: WOS:000455608400001

Author Identifiers:

Author	Web of Science ResearcherID	ORCID Number
Rysavy, Petr		0000-0002-6597-6616

ISSN: 1384-5810

eISSN: 1573-756X

Record 231 of 235

Title: Electron-Spin Structure and Metal-Ligand Bonding in Open-Shell Systems from Relativistic EPR and NMR: A Case Study of Catalysts

Author(s): Bora, PL (Bora, Pankaj L.); Novotny, J (Novotny, Jan); Ruud, K (Ruud, Kenneth); Komorovsky, S (Komorovsky, Stanisla

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION **Volume:** 15 **Issue:** 1 **Pages:** 201-214 **DOI:** 10.1021/acs.jctc.8b009

Abstract: Electron and nuclear magnetic resonance spectroscopies are indispensable and powerful methods for investigating t structures of open shell systems. We demonstrate that the NMR and EPR parameters are extremely sensitive quantitative probe density around heavy-metal atoms and the metal ligand bonding. Using relativistic density-functional theory, we have analyzed spin density and the EPR and NMR parameters in paramagnetic iridium(II/IV) complexes with a PNP pincer ligand. As the magne compounds containing Sd transition metal(s) are heavily affected by spin-orbit coupling, relativistic effects must be included in used a recent implementation of the fully relativistic Dirac-Kohn-Sham (DKS) method employing the hybrid PBEO functional an calculate EPR parameters and hyperfine NMR shifts. The modulation of the metal-ligand bond by the trans substituent (-Cl or N) structure around the central metal atom and ligands are shown to be reflected in the "long-range" through-bond Fermi-contact ligand C-13 and H-1 hyperfine couplings. Interestingly, the hyperfine coupling constant of the ligand atom L (A(L)) bonded direc changes its sign because of the dominating role of the paramagnetic spin-orbit (PSO) term. Furthermore, the electronic g-shift a the ligand A(L) are shown to invert their signs when nitrogen is substituted for chlorine, reflecting the different formal metal oxi in metal-ligand bond character. A full understanding of the substituent effects is provided by using chemical bond concepts in c orbital (MO) theory analysis of the second-order perturbation theory expression for the EPR parameters. Our findings are easily containing d-block elements and beyond. Relativistic DFT calculations of magnetic-resonance parameters are expected to frequ experimental observations and the characterization of hitherto unknown unstable or exotic species.

Accession Number: WOS:000455558200020

PubMed ID: 30485092

Author Identifiers:

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Novotny, Jan	D-7676-2012	0000-0002-1203-9549
Ruud, Kenneth	E-5947-2010	0000-0003-1006-8482
Marek, Radek	D-6929-2012	0000-0002-3668-3523

ISSN: 1549-9618

eISSN: 1549-9626

Record 232 of 235

Title: Ab initio study of the theoretical strength and magnetism of the Fe-Pd, Fe-Pt and Fe-Cu nanocomposites

Author(s): Kana, T (Kana, Tomas); Zouhar, M (Zouhar, Martin); Cerny, M (Cerny, Miroslav); Sob, M (Sob, Mojmir)

Source: JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS **Volume:** 469 **Pages:** 100-107 **DOI:** 10.1016/j.jmmm.2018.08.027

Abstract: We studied the Fe-Pd, Fe-Pt and Fe-Cu nanocomposites formed by Fe nanowires embedded in the fcc Pd, Pt or Cu ma nanowires oriented along the [0 0 1] crystallographic direction. They replace second nearest neighbor atoms in the matrix. By m between the nanowires we arrived to the chemical compositions X15Fe, X8Fe and X7Fe where X stands for Pd, Pt and Cu. The m properties of the nanocomposites were obtained by ab initio simulations. We performed tensile and compressive tests along th compared the results with the deformation behavior of the fcc matrix and the known intermetallic compounds FePd3 and FePt3 maximum attainable stress for the Fe-Pd and Fe-Pt nanocomposites is higher than the stress attainable for the Pd and Pt matric increased with the increasing Fe content. The increase was due to the enhanced stability in the nanocomposites described by tl This effect was particularly pronounced in the Fe-Pt nanocomposites. On the contrary, the Fe nanowires in the Fe-Cu nanocomp stability and strength of the Cu matrix. They even make the Cu matrix more compliant to compression. Regarding the magnetic Fe-Pt nanocomposites prefer a ferromagnetic configuration where the spins of all Fe atoms are oriented in parallel manner. On nanocomposites exhibit an antiferromagnetic configuration where the spins of all Fe atoms assigned to a particular nanowire a antiparallel to the spins of a neighboring Fe nanowire. The Young modulus E-001 along the [0 0 1] crystallographic direction inc content in both the Fe-Pd and Fe-Pt nanocomposites.

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Record 233 of 235

Title: Effect of a realistic three-body force on the spectra of medium-mass hypernuclei

Author(s): Vesely, P (Vesely, P.); De Gregorio, G (De Gregorio, G.); Pokorny, J (Pokorny, J.)

Source: PHYSICA SCRIPTA **Volume:** 94 **Issue:** 1 **Article Number:** 014006 **DOI:** 10.1088/1402-4896/aaecfa **Published:** JAN 2019

Abstract: We adopt the Hartree-Fock method in the proton-neutron-A formalism and the nucleon-A Tamm-Dancoff approximat spectra of medium-mass hypernuclei. The formalism is developed for a potential derived from effective field theories which inc NNN forces plus the YN LO potential. The energy spectra of selected medium-mass hypernuclei are presented and their propert calculation is the first step of a project devoted to ab initio studies of hypernuclei in medium and heavy mass regions. This may understanding of the YN interactions at momentum scales not accessible in few-body hypernuclei.

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Record 234 of 235

Title: Fast In Vivo High-Resolution Diffusion MRI of the Human Cervical Spinal Cord Microstructure

Author(s): Labounek, R (Labounek, Rene); Valosek, J (Valosek, Jan); Zimolka, J (Zimolka, Jakub); Piskorova, Z (Piskorova, Zuzar Svatkova, A (Svatkova, Alena); Bednarik, P (Bednarik, Petr); Hok, P (Hok, Pavel); Vojtisek, L (Vojtisek, Lubomir); Hlustik, P (Hlusti (Bednarik, Josef); Lenglet, C (Lenglet, Christophe)

Edited by: Lhotska L; Sukupova L; Lackovic I; Ibbott GS

Source: WORLD CONGRESS ON MEDICAL PHYSICS AND BIOMEDICAL ENGINEERING 2018, VOL 1 **Book Series:** IFMBE Proceeding 3-7 **DOI:** 10.1007/978-981-10-9035-6_1 **Published:** 2019

Abstract: Diffusion Magnetic Resonance Imaging (dMRI) is a widely-utilized method for assessment of microstructural propertie system i.e., the brain and spinal cord (SC). In the SC, almost all previous human studies utilized Diffusion Tensor Imaging (DTI), model areas where white matter (WM) pathways cross or diverge. While High Angular Diffusion Resolution Imaging (HARDI) can limitations, longer acquisition times critically limit its applicability to clinical human studies. In addition, previous human HARI spatial resolution, with typically a few slices and voxel size similar to 1 x 1 x 5 mm(3) being acquired in tens of minutes. Thus, we HARDI protocol that allows collecting dMRI data at high angular and spatial resolutions in clinically-feasible time. Our data was Prisma scanner, in less than 9 min. It has a total of 75 diffusion-weighted volumes and high spatial resolution of 0.67 x 0.67 x 3 m Fourier space) covering the cervical segments C4-C6. Our preliminary results demonstrate applicability of our technique in heal correspondence between low fractional anisotropy (FA) gray matter areas from the dMRI scans, and the same regions delineate with spatial resolution of 0.35 x 0.35 x 2.5 mm(3). Our data also allows the detection of crossing fibers that were previously shov studies.

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Record 235 of 235

Title: Stable EEG Spatiospectral Sources Using Relative Power as Group-ICA Input

Author(s): Labounek, R (Labounek, Rene); Bridwell, DA (Bridwell, David A.); Marecek, R (Marecek, Radek); Lamos, M (Lamos, Ma Brazdil, M (Brazdil, Milan); Jan, J (Jan, Jiri); Hlustik, P (Hlustik, Petr)

Edited by: Lhotska L; Sukupova L; Lackovic I; Ibbott GS

Source: WORLD CONGRESS ON MEDICAL PHYSICS AND BIOMEDICAL ENGINEERING 2018, VOL 2 **Book Series:** IFMBE Proceeding 125-128 **DOI:** 10.1007/978-981-10-9038-7_22 **Published:** 2019

Abstract: Within the last decade, various blind source separation algorithms (BSS) isolating distinct EEG oscillations were derive Independent Component Analysis (group-ICA) is a promising tool for decomposing spatiospectral EEG maps across multiple su are faced with many preprocessing options prior to performing group-ICA, which potentially influences the results. To examine preprocessing steps, within this article we compare results derived from group-ICA using the absolute power of spatiospectral r of spatiospectral maps. Within a previous study, we used K-means clustering to demonstrate group-ICA of absolute power spati sources which are stable across different paradigms (i.e. resting-state, semantic decision, visual oddball) Within the current stu with those obtained using relative power of spatiospectral maps as input to group-ICA. We find that relative EEG power contain patterns which were similar to those observed using absolute power as inputs. Interestingly, relative power revealed two c-ban were present across 3 paradigms, but not present using absolute power. This finding suggests that relative power potentially er which are obscured by the high energy low frequency which dominates absolute power measures.

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