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IN THIS ISSUE

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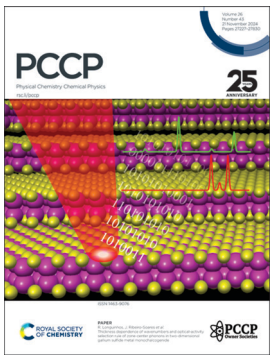


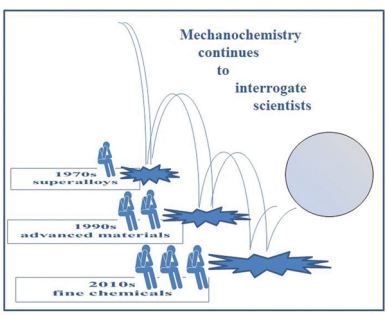
Cover
See R. Longuinhos, J. Ribeiro-Soares *et al.*, pp. 27260–27269. Image produced and designed by Raphael Longuinhos Monteiro Lobato, with the approval of the co-authors from *Phys. Chem. Chem. Phys.*, 2024, **26**, 27260.

EDITORIAL

27245

Fundamental basis of mechanochemical reactivity

Adam A. L. Michalchuk and Francesco Delogu

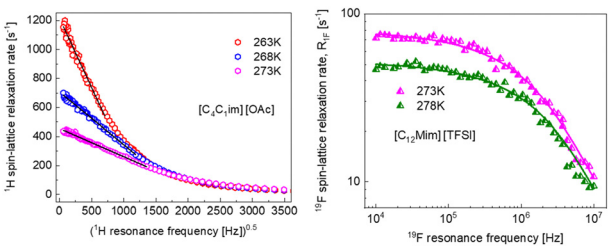


REVIEW

27248

Dynamics of ionic liquids by means of nuclear magnetic resonance relaxation – overview of theoretical approaches

Danuta Kruk,* Elzbieta Masiewicz, Roksana Markiewicz and Rajendra Kumar Singh



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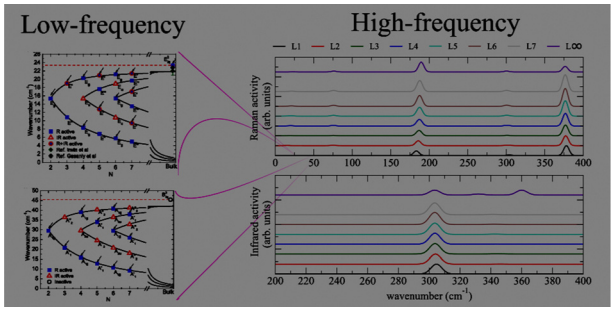
27260

Thickness dependence of wavenumbers and optical-activity selection rule of zone-center phonons in two-dimensional gallium sulfide metal monochalcogenide

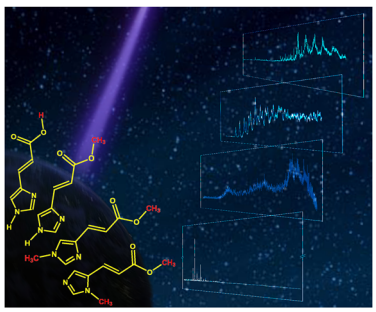
R. Longuinhos,* Dattatray J. Late, B. C. Viana, R. S. Alencar, M. Terrones, A. G. Souza Filho, A. Jorio and J. Ribeiro-Soares*



27270

Urocanic acid as a novel scaffold for next-gen nature-inspired sunscreens: I. electronic laser spectroscopy under isolated conditions

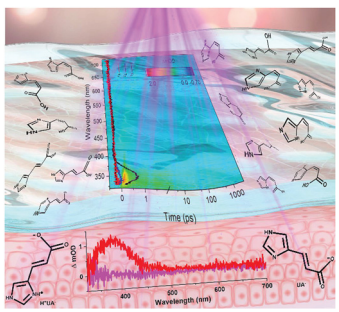
Jiayun Fan, Alexander K. Lemmens, Hans Sanders, Michiel Hilbers, Wim Roeterdink and Wybren Jan Buma*



27281

Urocanic acid as a novel scaffold for next-gen nature-inspired sunscreens: II. Time-resolved spectroscopy under solution conditions

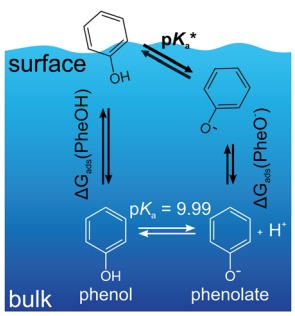
Jiayun Fan, Jack M. Wooley, Hans Sanders, Vasilios G. Stavros* and Wybren Jan Buma*



27292

Surface accumulation and acid–base equilibrium of phenol at the liquid–vapor interface

Clemens Richter,* Rémi Dupuy, Florian Trinter, Tillmann Buttersack, Louisa Cablitz, Shirin Gholami, Dominik Stemer, Christophe Nicolas, Robert Seidel, Bernd Winter and Hendrik Bluhm*



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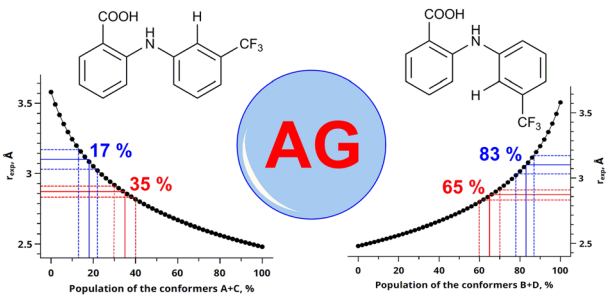
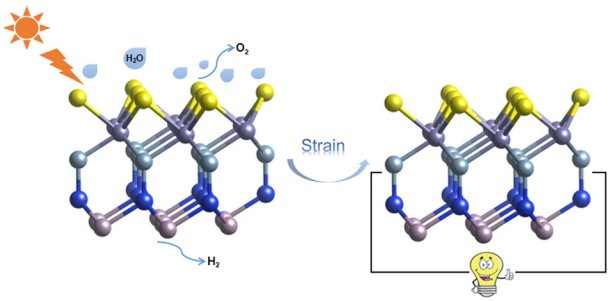


Structural and sorption characteristics of an aerogel composite material loaded with flufenamic acid: insights from MAS NMR and high-pressure NOESY studies

Valentina V. Sobornova, Valeriya V. Mulloyarova, Konstantin V. Belov, Alexey A. Dyshin, Peter M. Tolstoy, Mikhail G. Kiselev and Ilya A. Khodov*

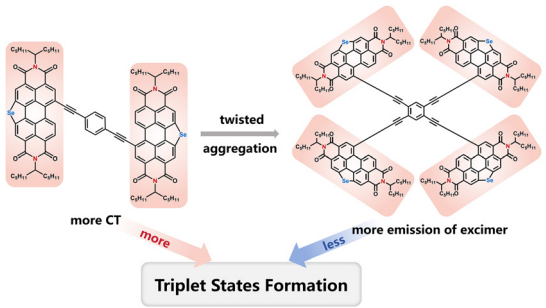
27314



Two-dimensional Janus XWZAZ′ (X = S, Se, Te; A = Si, Ge; Z, Z′ = N, P, As): candidates for photocatalytic water splitting and piezoelectric materials

Zhen Gao, Hongbo Wu, Yao He* and Kai Xiong*

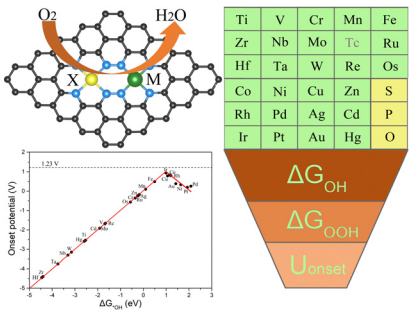
27325



The efficient triplet states formation of Se-modified PDI dimers and tetramers in solvents

Feijun Huang, Wenli Su, Yubo Yang, Hang Wang, Zhishan Bo, Pengfei Jing and Wenkai Zhang*

27332



Theoretical screening of the metal-nonmetal pair anchored on N-doped graphene for the oxygen reduction reaction

Ji Zhang, Peng Zhang, Aimin Yu, Dong-sheng Li and Chenghua Sun*

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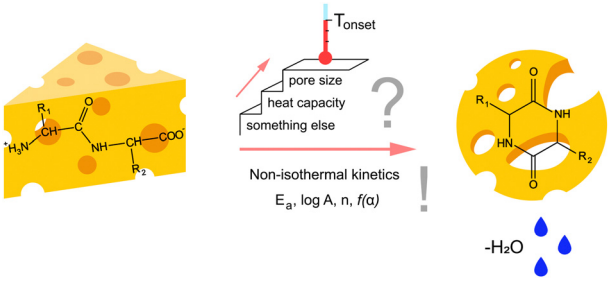
27338

Cyclization of alanyl–valine dipeptides in the solid state. The effects of molecular radiator and heat capacity

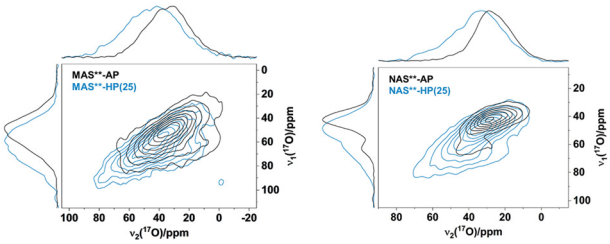
Daria V. Tkachenko, Radik A. Larionov, Sufia A. Ziganshina, Khasan R. Khayarov, Aleksandr E. Klimovitskii, Olga B. Babaeva, Valery V. Gorbatchuk and Marat A. Ziganshin*



27348

Densification of sodium and magnesium aluminosilicate glasses at ambient temperature: structural investigations by solid-state nuclear magnetic resonance and molecular dynamics simulations

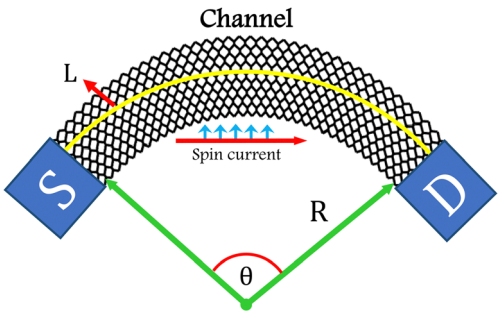
Millena Logrado, Yara Hellen Firmo Gomes, Tomiki Inoue, Shingo Nakane, Yoshinari Kato, Hiroki Yamazaki, Akihiro Yamada and Hellmut Eckert*



27363

Spintronic performance of bent zigzag phosphorene nanoribbons: effects of mechanical deformation and gate voltage

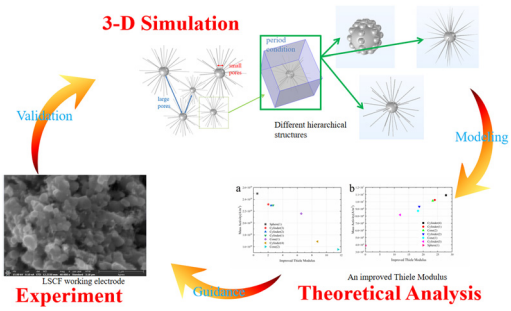
Rouhollah Farghadan



27371

Strategy for predicting catalytic activity of catalysts with hierarchical nanostructures

Zidi Zhu, Daoming Huan, Jingchao Yuan, Dan Zhang,* Aijun Li and Jiujun Zhang



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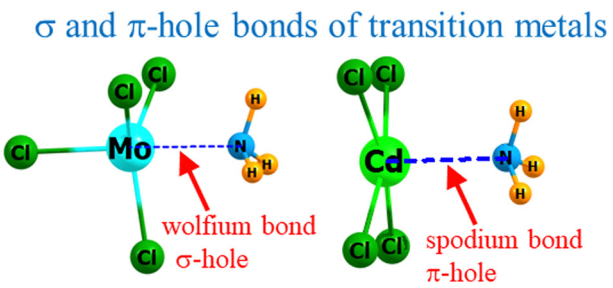
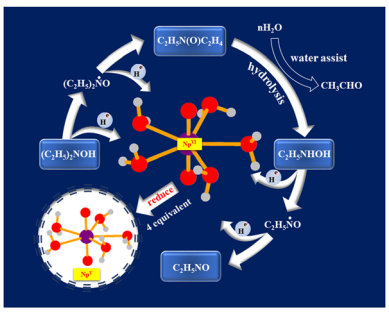


Participation of transition metal atoms in noncovalent bonds

Steve Scheiner

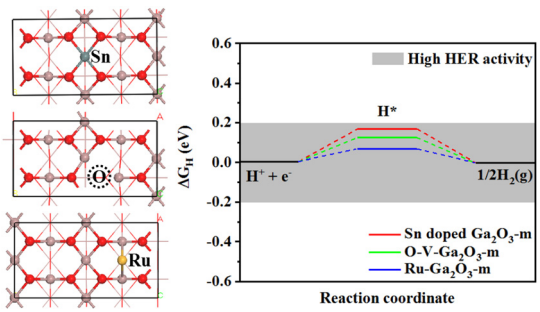
27395



Uncovering the reduction mechanism of Np(VI) with *N,N*-diethyl hydroxylamine: a scalar-relativistic DFT investigation

Xin Huang, Xiaobo Li, Qunyan Wu,* Congzhi Wang, Jianhui Lan, Hongqing Wang and Weiqun Shi*

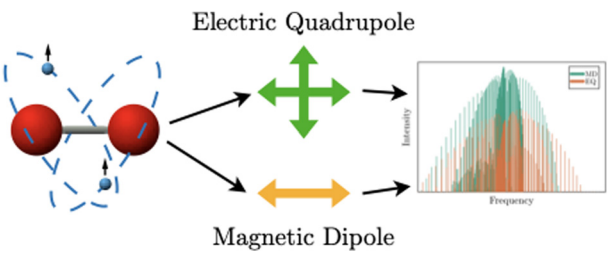
27406



Theoretical design of active Ga_2O_3 monolayer-based catalysts for electrocatalytic HER

Rongzhi Wang and Jin-Cheng Zheng*

27419



An *ab initio* spectroscopic model of the molecular oxygen atmospheric and infrared bands

Wilfrid Somogyi,* Sergey N. Yurchenko and Gap-Sue Kim

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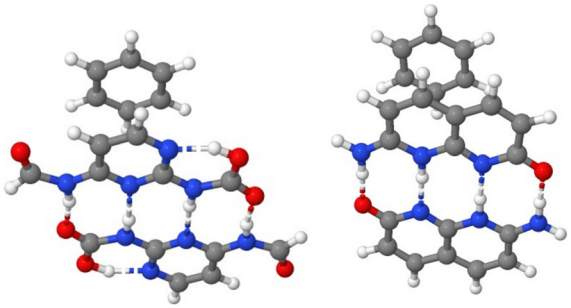
The effect of hydrogen bonding on the π depletion and the π–π stacking interaction

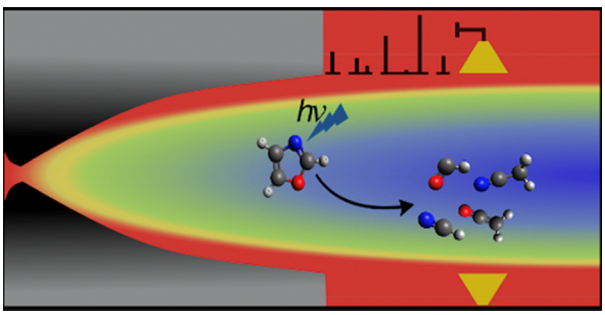
Usman Ahmed, Dage Sundholm* and Mikael P. Johansson*



27439

Product branching in the photodissociation of oxazole detected by broadband rotational spectroscopy

Briony Downes-Ward, Abbas Behzadfar, Shameemah Thawoos and Arthur G. Suits*



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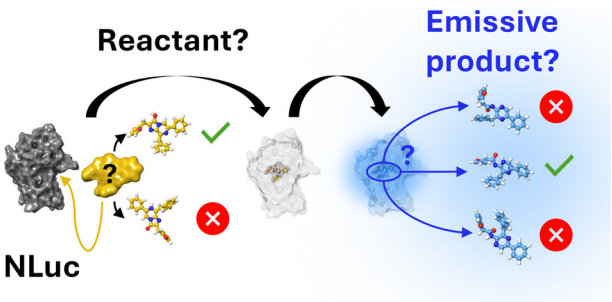
Behind the glow: unveiling the nature of NanoLuc reactants and products

Alessandro Bonardi, Michele Turelli, Giorgio Moro, Claudio Greco, Ugo Cosentino* and Carlo Adamo*



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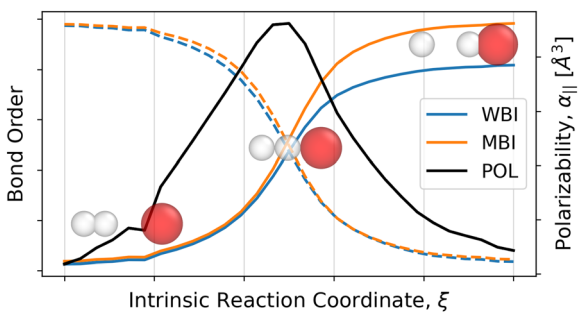
Near equivalence of polarizability and bond order flux metrics for describing covalent bond rearrangements

Lukas Kim and Teresa Head-Gordon*



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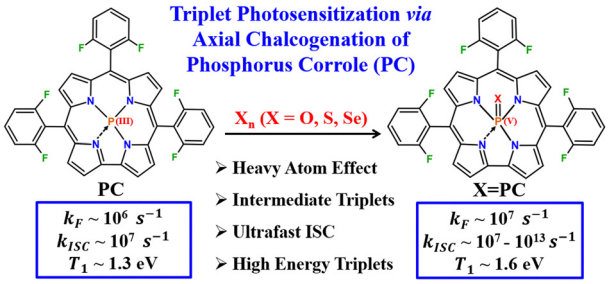
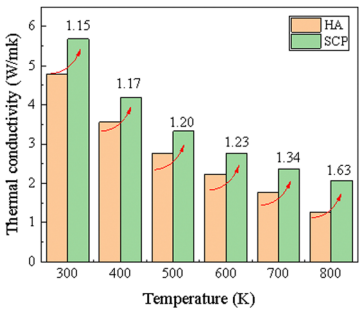


Tailoring intersystem crossing in phosphorus corroles through axial chalcogenation: a detailed theoretical study

Annette Mariya Tedy and Arun K. Manna*

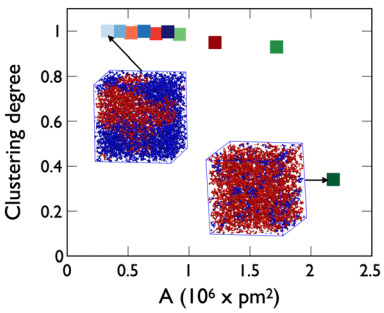
27478



Thermal conductivity study of 2D Si_4C_8 materials by anharmonic phonon renormalization

Peng Gao, Xihao Chen,* Xingwu Yan, Longxin Zhang, Xiang Meng, Fuqiang Zhai* and Donglin Guo*

27486



Structural insights into carboxylic-acid based DES across H-bond donor ratios: impact of CL&Pol refinement

Jon Zubeltzu* and Elixabete Rezabal

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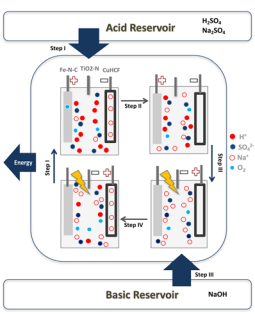

Electrochemical system of nitrogen-doped TiO_2, Fe–N–C, and copper hexacyanoferrate electrodes for photo-assisted energy conversion in acidic wastewater treatment

Bianca Tainá Ferreira, Matheus Martins and Fritz Huguenin*

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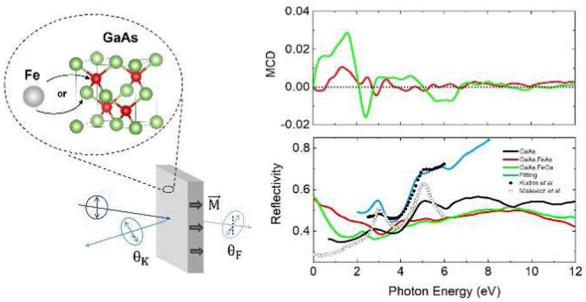
RESEARCH PAPERS

27510

Magneto-optical properties of heavily Fe-doped GaAs: a density functional approach

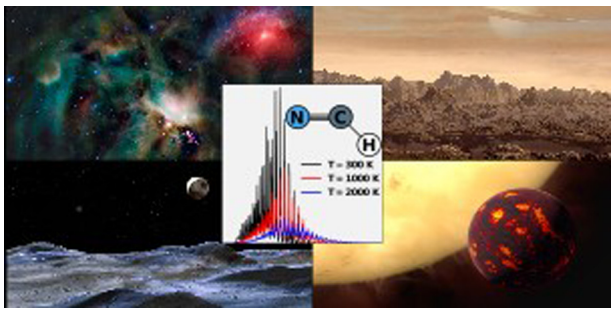
J. Zarpellon,* D. H. Mosca and J. Varalda



27519

A time-independent, variational method for studying the photodissociation of triatomic molecules

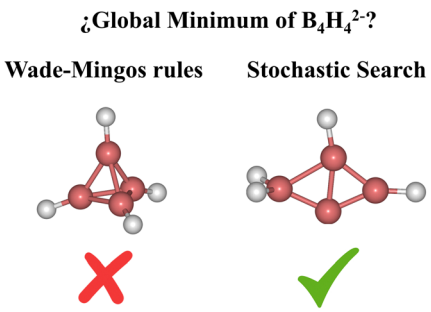
Marco Pezzella, Georgi Mitev, Sergei N. Yurchenko, Jonathan Tennyson* and Alexander O. Mitrushchenkov



27530

Exploring the potential energy surface of $B_4H_4^{2-}$: an exception of the Wade–Mingos rules

Rodrigo Báez-Grez, Alejandro Vásquez-Espinal* and Ricardo Pino-Rios*



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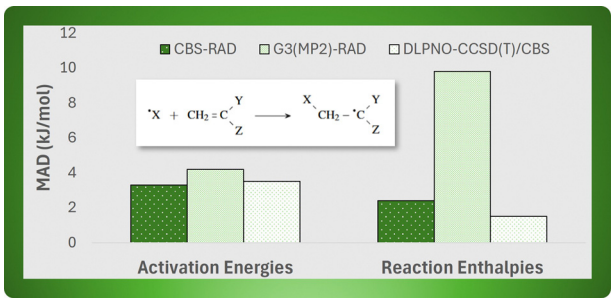
Comparing coupled cluster and composite quantum chemical methods for computing activation energies and reaction enthalpies of radical propagation reactions

Timothy B. Huber* and Ralph A. Wheeler*



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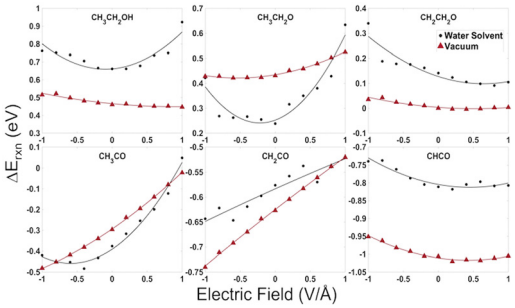
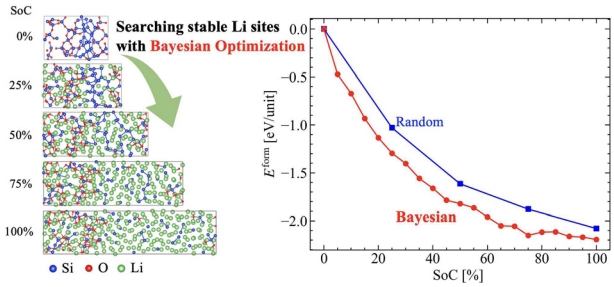


Modeling interfacial electric fields and the ethanol oxidation reaction at electrode surfaces

Yuhan Mei, Fanglin Che and N. Aaron Deskins*

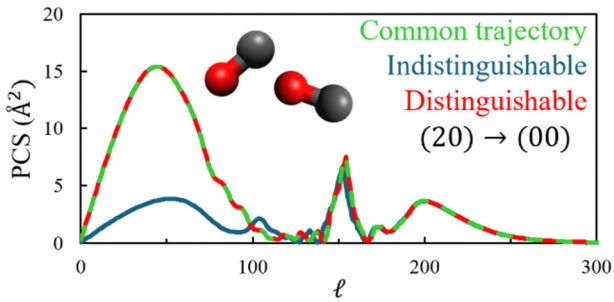
27561



First-principles study on the lithiation process of amorphous SiO anode for Li-ion batteries with Bayesian optimization

Ryoya Shintaku, Tomoyuki Tamura,* Shogo Nogami, Masayuki Karasuyama and Takakazu Hirose

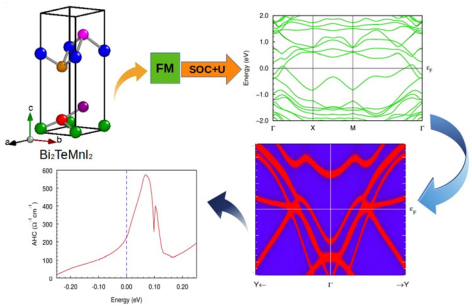
27567



Mixed quantum/classical theory for rotationally inelastic scattering of identical collision partners revised

D. Bostan, B. Mandal and D. Babikov*

27583



Emergence of Weyl points and large anomalous Hall conductivity in layered Bi_2TeMnI_2

Dipak Bhattarai, Deergh Bahadur Shahi, Dipendra Prasad Kalauni and Madhav Prasad Ghimire*

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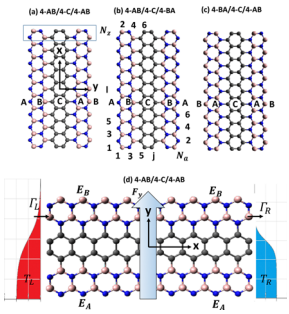
Impact of valley degeneracy on the thermoelectric properties of zig-zag graphene nanoribbons with staggered sublattice potentials and transverse electric fields

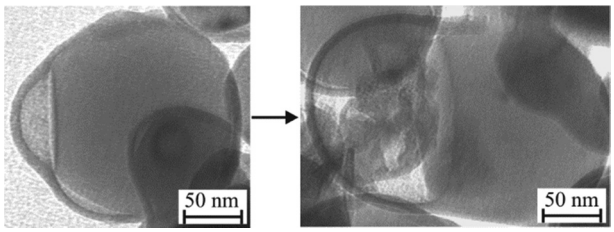
David M. T. Kuo



27602

Oxidation of fine aluminum particles: thermally induced transformations in particle shells and kinetics of oxide nucleation

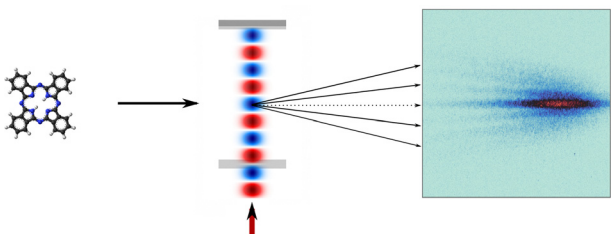
Andrey V. Korshunov



27617

Diffracting molecular matter-waves at deep-ultraviolet standing-light waves

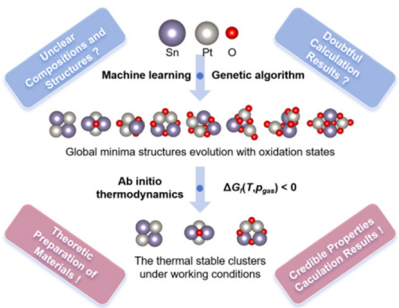
Ksenija Simonović,* Richard Ferstl, Alfredo Di Silvestro, Marcel Mayor, Lukas Martinetz, Klaus Hornberger, Benjamin A. Stickler, Christian Brand and Markus Arndt



27624

Machine-learning-accelerated structure prediction of PtSnO nanoclusters under working conditions

Fanke Zeng and Wanglai Cen*



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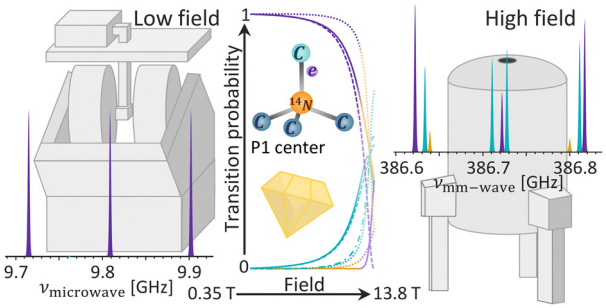
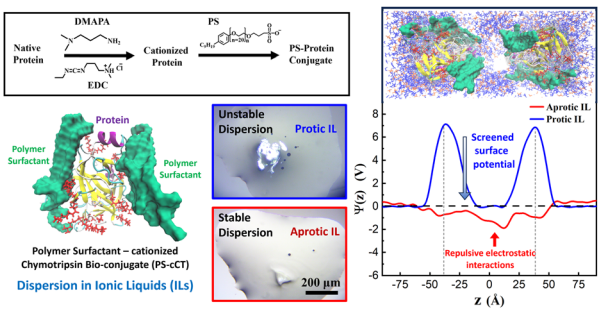
27633



On the peculiar EPR spectra of P1 centers at high (12–20 T) magnetic fields

Orit Nir-Arad, Eyal Laster, Mais Daksi, Nurit Manukovsky and Ilia Kaminker*

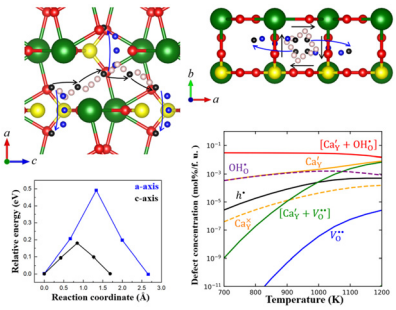
27648



Cation effects and charge inversion contribute to the electrostatic stabilisation of protein bioconjugates in neat ionic liquids

Lokesh Soni, Raj Kumar, Kamendra P. Sharma* and Ajay Singh Panwar*

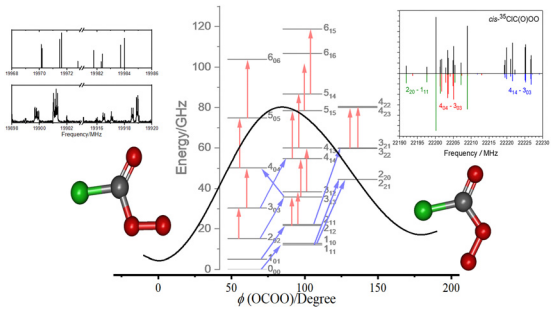
27660



First-principles calculations of proton defect properties in Ca-doped YPO_4

Gyeongseo Lee,* Takafumi Ogawa, Kazuki Shitara and Akihide Kuwabara*

27669



Insights of the peroxychloroformyl radical ClC(O)OO *via* microwave spectrum

Ching-Hua Chang, Wen Chao, Cheng-Han Tsai, Mitchio Okumura, Frank A. F. Winiberg and Yasuki Endo*

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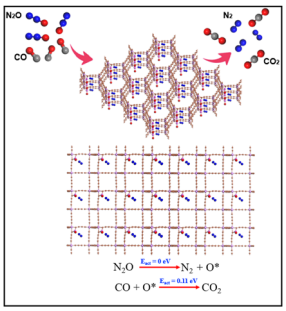
27677

Unveiling the potential of aluminum-decorated 3D phosphorus graphdiyne as a catalyst for N_2O reduction

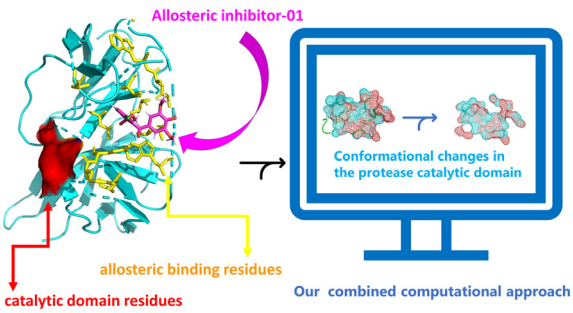
Shehzad Ahmed, Adnan Ali Khan,* Danish Khan, Awais Ghani,* Rashid Ahmad, Tian Xiaoqing* and Imran Muhammad*



27684

***In silico* validation of allosteric inhibitors targeting Zika virus NS2B–NS3 protease**

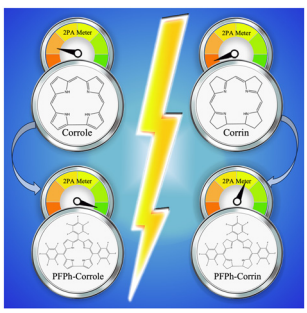
Yeng-Tseng Wang,* Yuan-Chin Hsieh and Tin-Yu Wu



27694

Effect of *meso*-pentafluorophenyl group on two-photon absorption in heterocorroles and heterocorrins

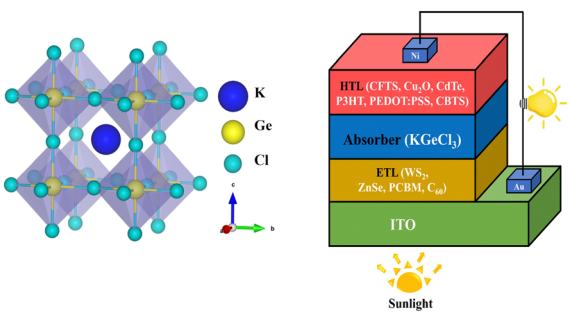
Tejendra Banana, Swati Singh Rajput, Neelam Chandravanshi and Md. Mehboob Alam*



27704

An in-depth investigation of lead-free $KGeCl_3$ perovskite solar cells employing optoelectronic, thermomechanical, and photovoltaic properties: DFT and SCAPS-1D frameworks

Md. Tarekuzzaman, Mohammad Hasin Ishraq, Md. Shahazan Parves, M. A. Rayhan, Sohail Ahmad, Md. Rasheduzzaman, K A Al Mamun, M. Moazzam Hossen and Md. Zahid Hasan*



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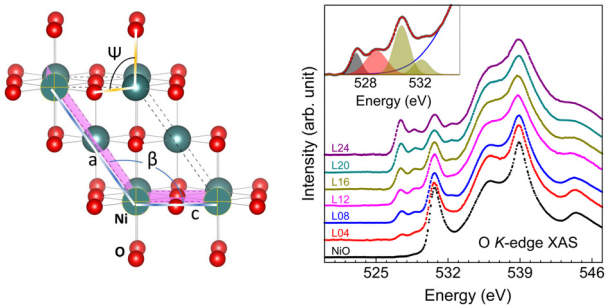
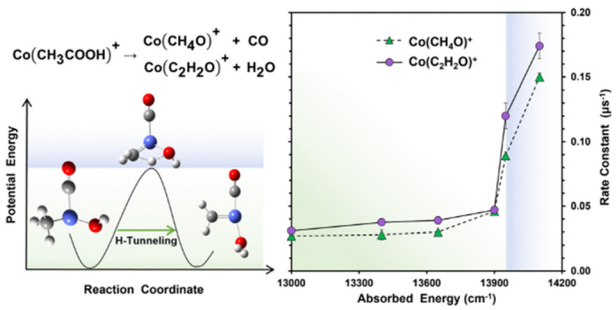
27735



Hole-states in Li doped NiO: doping dependence of Zhang-Rice spectral weight

Suman Mandal* and Krishnakumar S. R. Menon

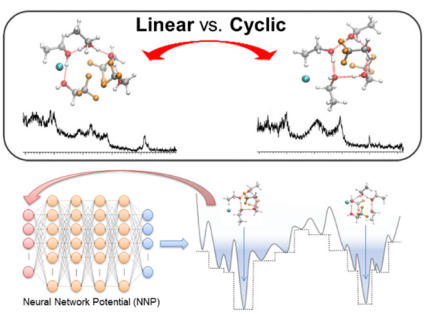
27741



Hydrogen tunneling with an atypically small KIE measured in the mediated decomposition of the $Co(CH_3COOH)^+$ complex

Simon U. Okafor, Gabriele Pinto, Michael Brdecka, William Smith, Tucker W. R. Lewis, Michael Gutierrez and Darrin J. Bellert*

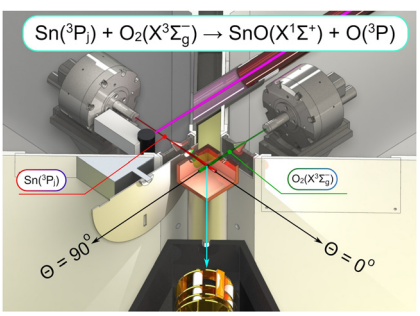
27751



Hydrogen bond network structures of protonated 2,2,2-trifluoroethanol/ethanol mixed clusters probed by infrared spectroscopy combined with a deep-learning structure sampling approach: the origin of the linear type network preference in protonated fluoroalcohol clusters

Po-Jen Hsu, Atsuya Mizuide, Jer-Lai Kuo* and Asuka Fujii*

27763



Experimental and theoretical study of the Sn–O bond formation between atomic tin and molecular oxygen

Iakov A. Medvedkov, Anatoliy A. Nikolayev, Shane J. Goettl, Zhenghai Yang, Alexander M. Mebel* and Ralf I. Kaiser*

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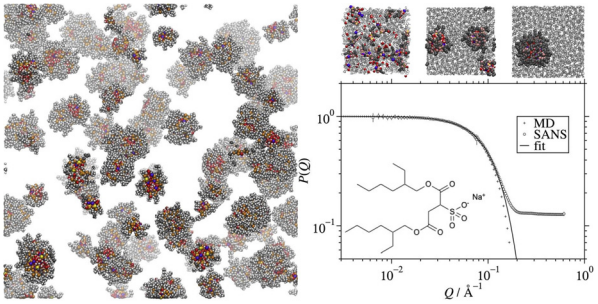
27772

Experimental and simulation study of reverse micelles formed by aerosol-OT and water in non-polar solvents

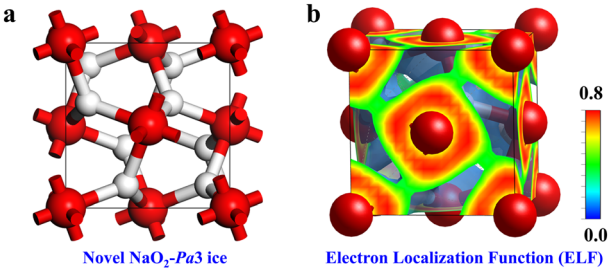
Angie Mat'usová, Georgina Moody, Peter J. Dowding, Julian Eastoe and Philip J. Camp*



27783

New metallic ice phase under high pressure

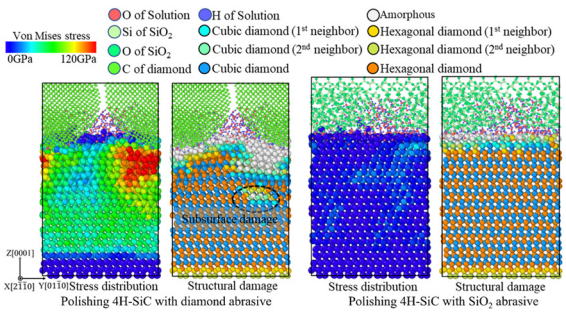
Yingying Huang,* Liuyuan Zhu, Hanlin Li, Haiping Fang, Ruoyang Chen* and Shiqi Sheng*



27791

Effects of oxidizer concentration and abrasive type on interfacial bonding and material removal in 4H-SiC polishing processes

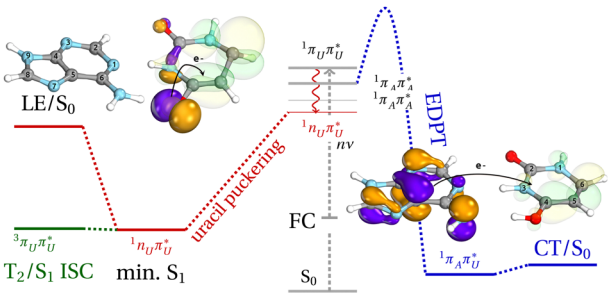
Yuqi Zhou, Kezhong Xu, Yuhan Gao, Ziniu Yu and Fulong Zhu*



27807

Theoretical insight into photodeactivation mechanisms of adenine–uracil and adenine–thymine nucleobase pairs

Kinga Szkaradek* and Robert W. Góra*



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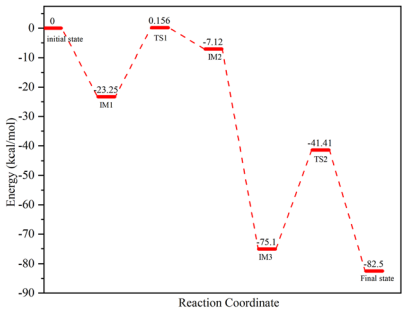

Performance of functionalized graphene oxide with organic radical scavengers in proton exchange membranes

Yu Hu, Jiaxing Wang, Shuai Wang* and Yuan Feng

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