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ISSN 1463–9076 CODEN PPCPFQ 26(17) 12897–13516 (2024)

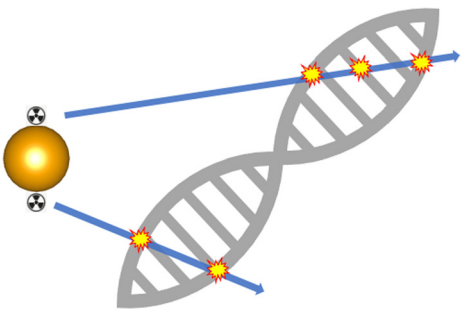
Cover
See Lai-Sheng Wang *et al.*, pp. 12928–12938. Image reproduced by permission of Ivan Popov from *Phys. Chem. Chem. Phys.*, 2024, **26**, 12928.

TUTORIAL REVIEW

12915

^{211}At on gold nanoparticles for targeted radionuclide therapy application

Jeffrey Tanudji, Hideaki Kasai,* Michio Okada, Tetsuo Ogawa, Susan M. Aspera and Hiroshi Nakanishi

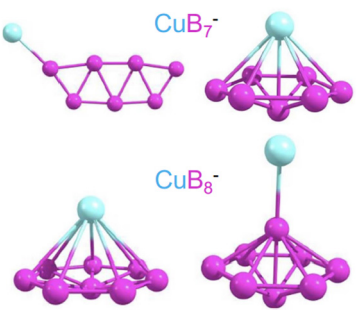


RESEARCH PAPERS

12928

Searching for stable copper borozene complexes in CuB_7^- and CuB_8^-

Wei-Jia Chen, Anton S. Pozdeev, Hyun Wook Choi, Alexander I. Boldyrev, Dao-Fu Yuan,* Ivan A. Popov* and Lai-Sheng Wang*



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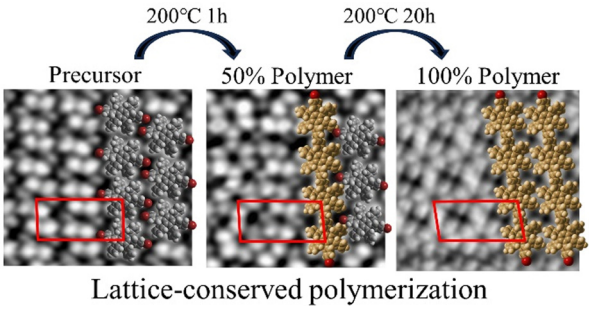
12939

On-surface polymerization reactions of dibrominated hexaphenylbenzene influenced by densely packed self-assembly

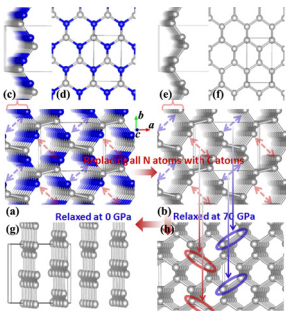
Hiroaki Ooe and Takashi Yokoyama*



12947

Prediction of superhard $C_{1+x}N_{1-x}$ compounds with metal-free magnetism and narrow band gaps

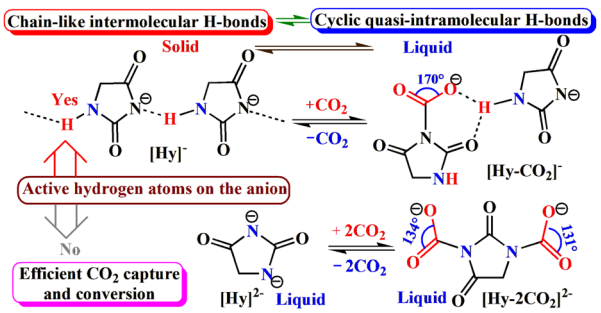
Haiping Wu,* Yunhao Zheng, Erjun Kan and Yan Qian*



12957

Does the active hydrogen atom in the hydantoin anion affect the physical properties, CO_2 capture and conversion of ionic liquids?

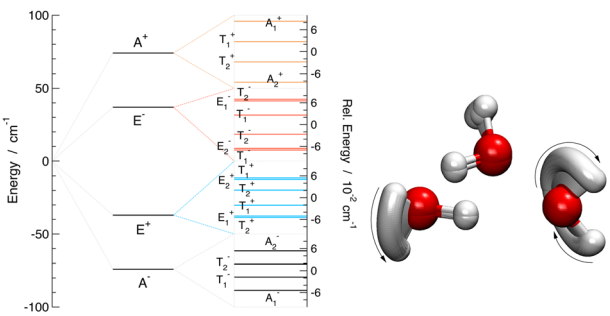
Tingting Chen, Zhongyuan Sun, Yujun Guo and Yingjie Xu*



12965

Tunneling splittings in the vibrationally excited states of water trimer

Mihael Eraković and Marko T. Cvitaš*



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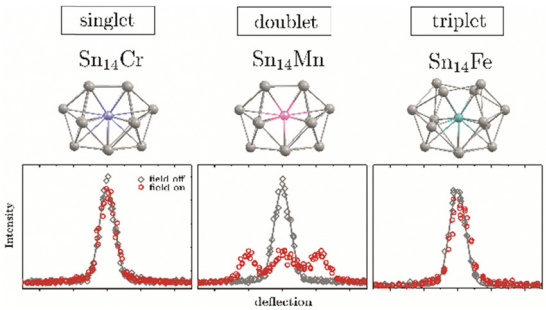
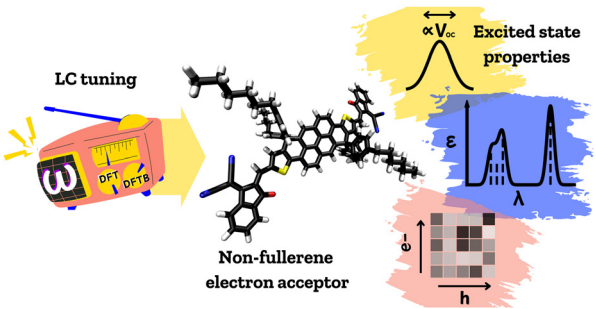


Magnetism of single-doped paramagnetic tin clusters studied using temperature-dependent Stern–Gerlach experiments with enhanced sensitivity: impact of the diamagnetic ligand field and paramagnetic dopant

Filip Rivic* and Rolf Schäfer

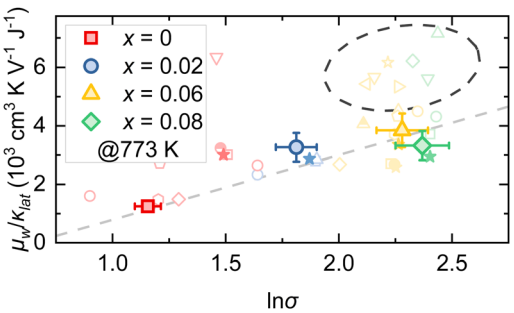
12993



Excited state properties of an A–D–A non-fullerene electron acceptor: a LC-TD-DFTB study

R. B. Ribeiro* and M. T. do N. Varella

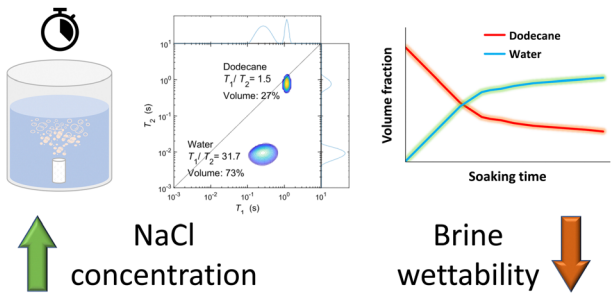
13006



Thermoelectric properties of $Bi_{1-x}Pb_xCu_{1-x}SeO$ oxyselenides

Aleksandra Khanina,* Andrei Novitskii, Daria Pashkova, Andrei Voronin, Takao Mori and Vladimir Khovaylo*

13012



Investigating the behaviour of NaCl brines and hydrocarbons in porous alumina using low-field NMR relaxation and diffusion methods

Aristarchos Mavridis, Mark Sankey, Kuhan Chellappah and Carmine D'Agostino*

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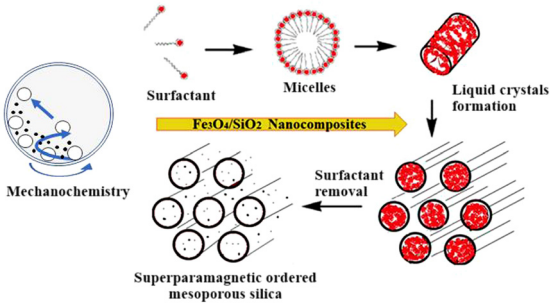
13020

Combining high energy ball milling and liquid crystal templating method to prepare magnetic ordered mesoporous silica. A physico-chemical investigation

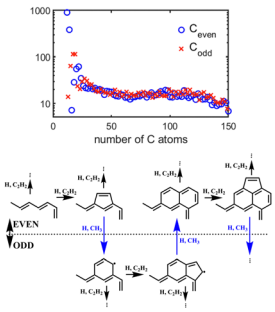
Alessandra Scano,* Edmond Magner, Martina Pilloni, Luciano Atzori, Marzia Fantauzzi, Sawssen Slimani, Davide Peddis, Gonzalo Garcia Fuentes and Guido Ennas



13034

Phenalenyl growth reactions and implications for prenucleation chemistry of aromatics in flames

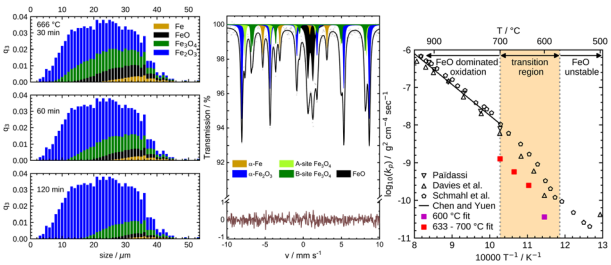
Michael Frenklach,* Ahren W. Jasper and Alexander M. Mebel*



13049

Exploring the oxidation behavior of undiluted and diluted iron particles for energy storage: Mössbauer spectroscopic analysis and kinetic modeling

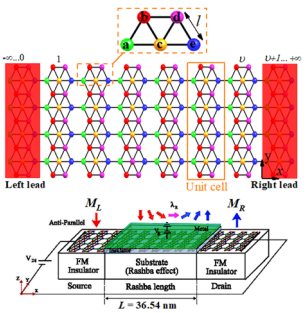
Jonas Spielmann, Daniel Braig, Antonia Streck, Tobias Gustmann, Carola Kuhn, Felix Reinauer, Alexandr Kurnosov, Oliver Leubner, Vasily Potapkin, Christian Hasse, Olaf Deutschmann, Bastian J. M. Etzold, Arne Scholtissek* and Ulrike I. Kramm*



13061

Ultrafast switching in spin field-effect transistors based on borophene nanoribbons

Farzaneh Ghasemzadeh, Mohsen Farokhnezhad* and Mahdi Esmaeilzadeh*



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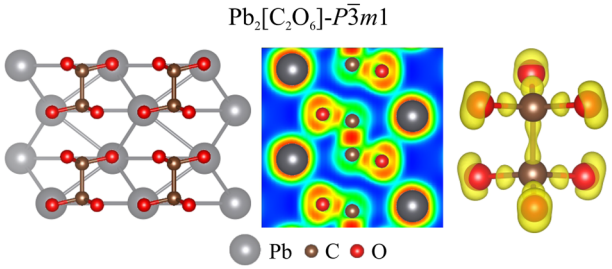
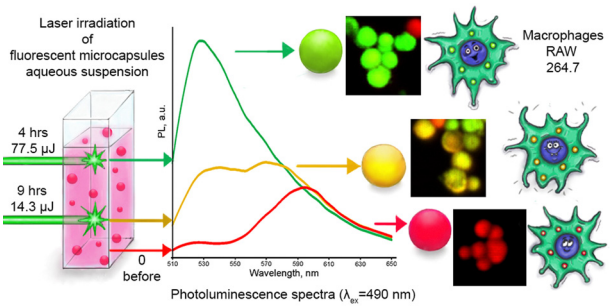
13070



$Pb_2[C_2O_6]$-$P\bar{3}m1$: new insights into the high-pressure behavior of carbonates

Maksim V. Banaev,* Dinara N. Sagatova,* Nursultan E. Sagatov and Pavel N. Gavryushkin

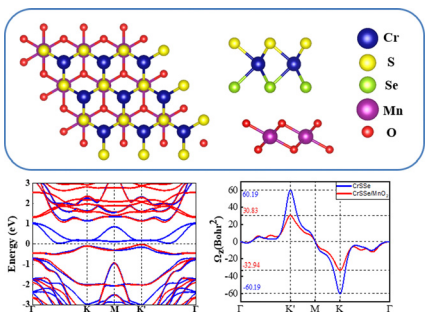
13078



Effect of photoconversion conditions on the spectral and cytotoxic properties of photoconvertible fluorescent polymer markers

Polina A. Demina,* Oleg V. Grishin, Sergey N. Malakhov, Olesya I. Timaeva, Elizaveta S. Kulikova, Timofey E. Pylaev, Mariia S. Saveleva and Irina Yu. Goryacheva

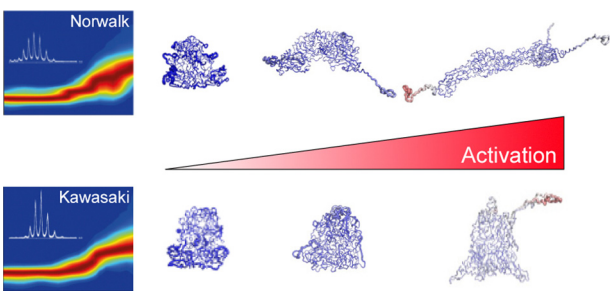
13087



Enhancement and modulation of valley polarization in Janus CrSSe with internal and external electric fields

Runxian Jiao, Qingyuan Wei, Lichuan Zhang, Yuee Xie, Jingjing He,* Yangbo Zhou,* Lei Shen and Jiaren Yuan*

13094



Collision induced unfolding and molecular dynamics simulations of norovirus capsid dimers reveal strain-specific stability profiles

Maxim N. Brodmerkel, Lars Thiede, Emiliano De Santis, Charlotte Uetrecht, Carl Caleman and Erik G. Marklund*

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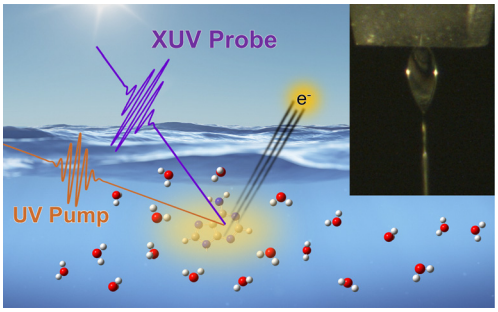
13106

Extreme ultraviolet time-resolved photoelectron spectroscopy of adenine, adenosine and adenosine monophosphate in a liquid flat jet

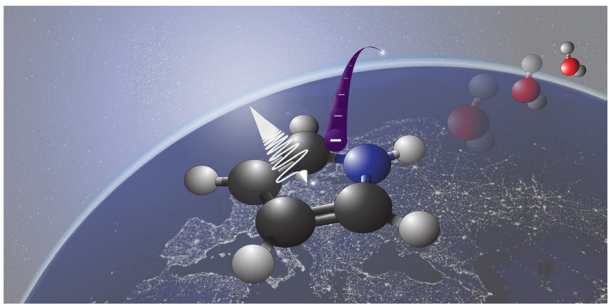
Masafumi Koga, Do Hyung Kang, Zachary N. Heim, Philipp Meyer, Blake A. Erickson, Neal Haldar, Negar Baradaran, Martina Havenith and Daniel M. Neumark*



13118

Water is a radiation protection agent for ionised pyrrole

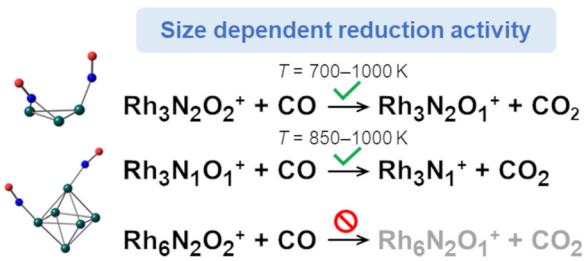
Melby Johny, Constant A. Schouder, Ahmed Al-Refaie, Lanhai He, Joss Wiese, Henrik Stapelfeldt, Sebastian Trippel* and Jochen Küpper



13131

Size-dependent reactivity of Rh cationic clusters to reduce NO by CO in the gas phase at high temperatures

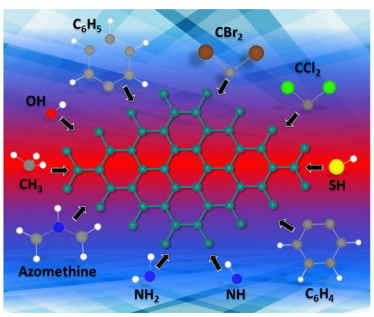
Ken Miyajima, Toshiaki Nagata, Fumitaka Mafuné,* Tomoya Ichino, Satoshi Maeda, Taizo Yoshinaga, Masahide Miura and Takahiro Hayashi



13140

Covalent functionalization of germanene employing computational simulations

Pablo A. Denis,* Jose A. S. Laranjeira and Julio R. Sambrano*



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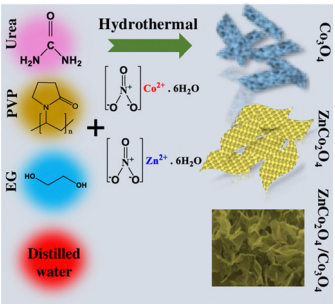
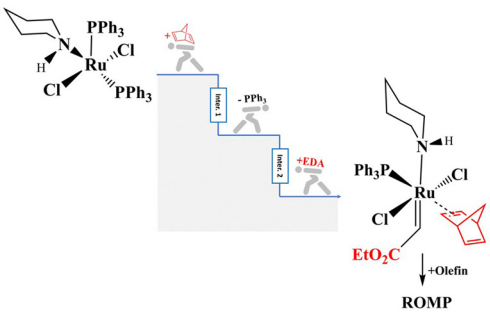


Synergistic effect between $ZnCo_2O_4$ and Co_3O_4 induces superior electrochemical performance as anodes for lithium-ion batteries

Anubha Tomar, Zulkifli, Jay Singh, Satendra Pal Singh, Jaekook Kim* and Alok Kumar Rai*

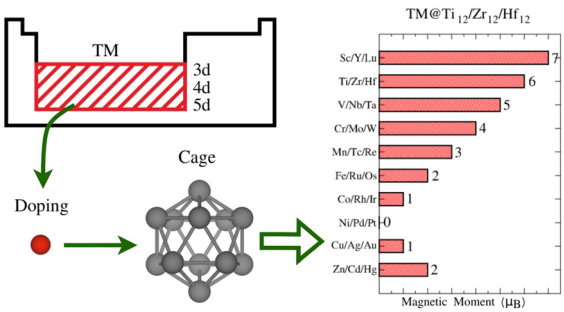
13164



Structural and thermodynamic insights into the coordination preference of norbornadiene with the initiator complex $[RuCl_2(PPh_3)_2(piperidine)]$ in polymerization *via* olefin metathesis

José Antonio de Sousa, José Luiz da Silva Sá, José Walkimar de Mesquita Carneiro and José Milton Elias de Matos*

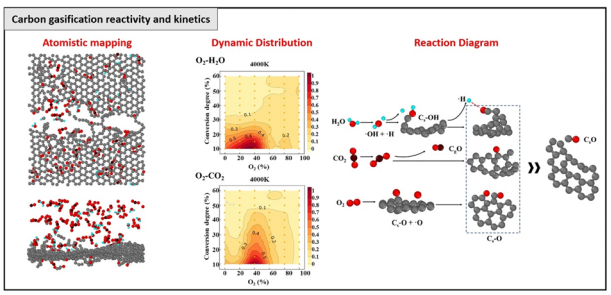
13172



Cage doping of Ti, Zr, and Hf-based 13-atom nanoclusters: two sides of the same coin

Maurício J. Piotrowski,* João Marcos T. Palheta and René Fournier*

13182



Interactions of graphene with oxidants in a mixed atmosphere: synergistic effects of O_2/H_2O and O_2/CO_2 on gasification reactivity and kinetics

Zeng Liang, Rita Khanna, Kejiang Li,* Yunfei Ma, Yuri Konyukhov, Yushan Bu, Jianliang Zhang and Alberto N. Conejo

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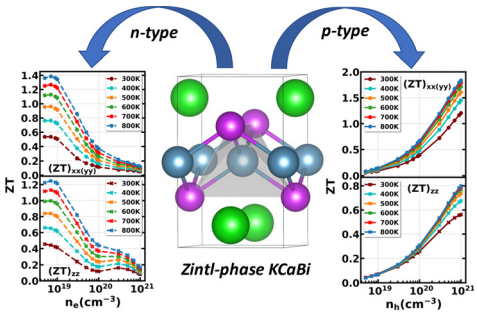
13198

Understanding the origin of the high thermoelectric figure of merit of Zintl-phase KCaBi

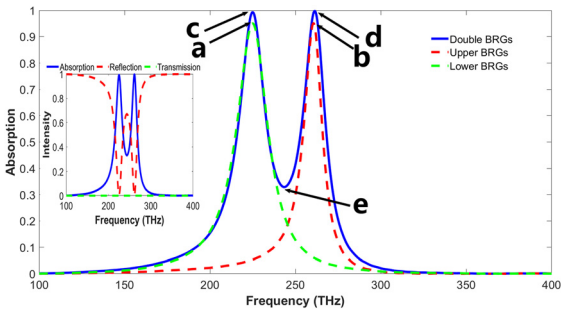
Sampad Mandal, Atish Ghosh and Pranab Sarkar*



13209

Dynamically tunable multi-band plasmon-induced absorption based on multi-layer borophene ribbon gratings

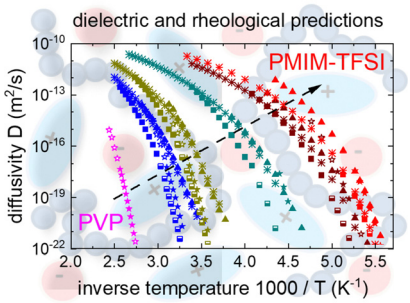
Yizhao Pan, Yuchang Li, Fang Chen,* Wenxing Yang and Zao Yi



13219

Relaxation and diffusion of an ionic plasticizer in amorphous poly(vinylpyrrolidone)

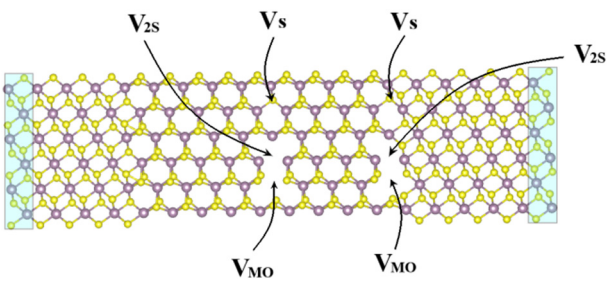
Lara Röwekamp, Kevin Moch,* Merve Seren, Philipp Münzner, Roland Böhmer and Catalin Gainaru



13230

Effect of point defects on the band alignment and transport properties of 1T-MoS_2/2H-MoS_2/1T-MoS_2 heterojunctions

Yifei Cong, Bairui Tao, Xinzhu Lu, Xiaojie Liu, Yin Wang and Haitao Yin*



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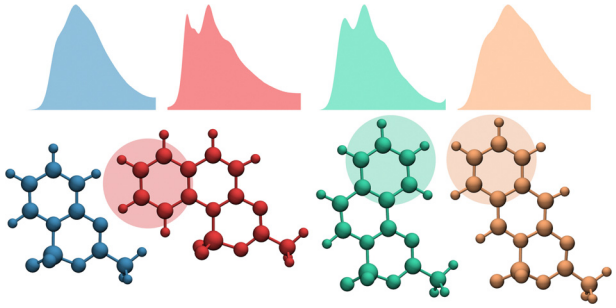
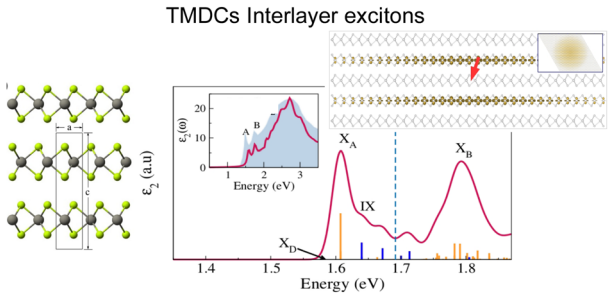


One- and two-photon absorption spectra of organoboron complexes: vibronic and environmental effects

Elizaveta F. Petrusevich, Heribert Reis, Borys Ośmiałowski, Denis Jacquemin, Josep M. Luis* and Robert Zaleśny*

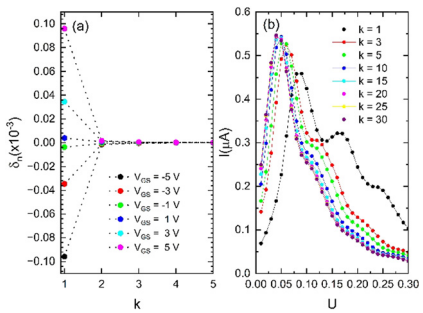
13251



Optical spectra and exciton radiative lifetimes in bulk transition metal dichalcogenides

Cesar E. P. Villegas,* Enesio Marinho Jr., Pedro Venezuela and Alexandre R. Rocha

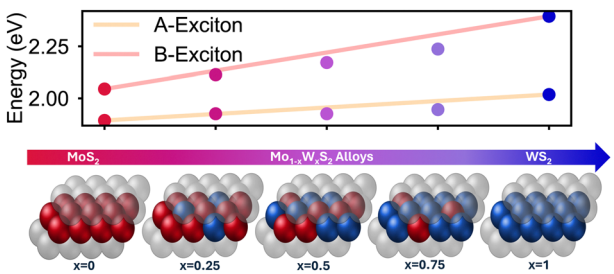
13261



Spin-polarized currents induced in antiferromagnetic polymer multilayered field-effect transistors

Shih-Jye Sun,* Miroslav Menšík and Petr Toman

13271



Colloidal 2D $Mo_{1-x}W_xS_2$ nanosheets: an atomic- to ensemble-level spectroscopic study

Markus Fröhlich, Marco Kögel, Jonas Hiller, Leo Kahlmeyer, Alfred J. Meixner, Marcus Scheele, Jannik C. Meyer and Jannika Lauth*

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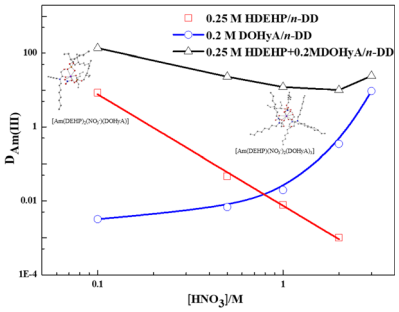
13279

Elucidation of the extraction of trivalent actinides using the DOHyA–HDEHP system: an experimental and theoretical approach

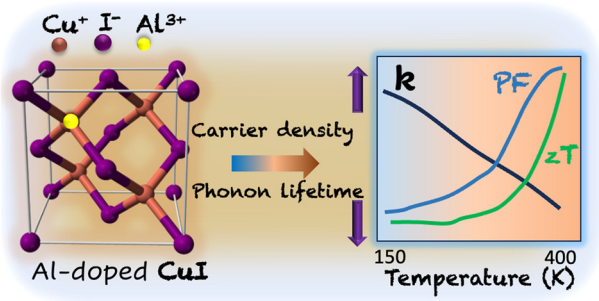
K. Rama Swami,* N. Parvathy, Abigail Jennifer G, Ramesh L. Gardas and Elumalai Varathan*



13287

Probing the thermoelectric properties of aluminium-doped copper iodide

Tatavarthi Veera Venkata Ramana,* Manjusha Battabyal,* Santosh Kumar, Dillip K. Satapathy* and Ravi Kumar*



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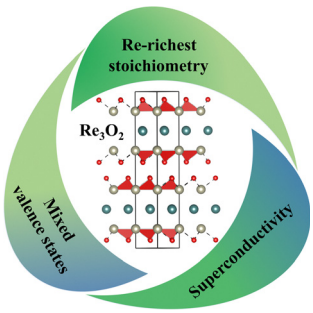
Metallic Re_3O_2 with mixed-valence states

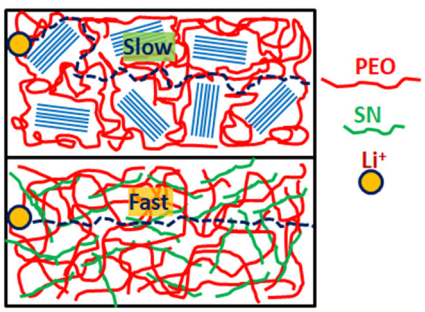
Wenjing Li, Fei Li,* Xiaohua Zhang, Jinhui Wu and Guochun Yang*



13306

Decoupling of ion-transport from polymer segmental relaxation and higher ionic-conductivity in poly(ethylene oxide)/succinonitrile composite-based electrolytes having low lithium salt doping

J. Mor and S. K. Sharma*



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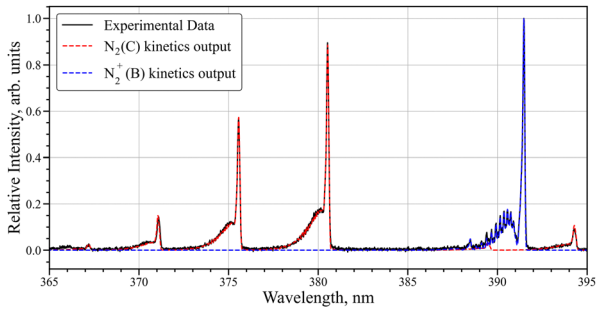
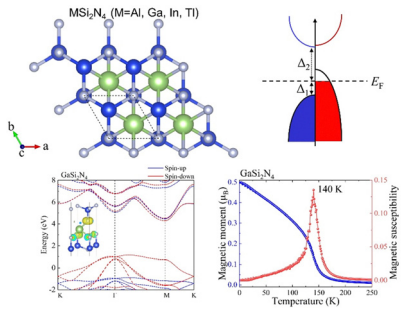


Spectral analysis and kinetic modeling of radioluminescence in air and nitrogen

E. R. Jans,* T. Casey, G. J. Marshall, C. M. Murzyn, S. S. Harilal, B. S. McDonald and R. K. Harrison

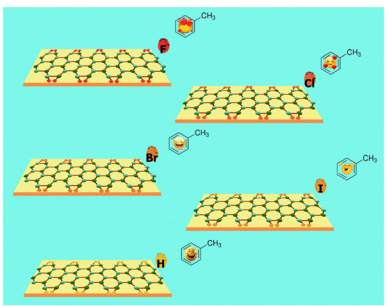
13327



Two-dimensional half-metals MSi_2N_4 (M = Al, Ga, In, Tl) with intrinsic p-type ferromagnetism and ultrawide bandgaps

Yi-min Ding,* Yiqi Huo, Gaojing Fang, Luo Yan, Yu Wu* and Liujiang Zhou*

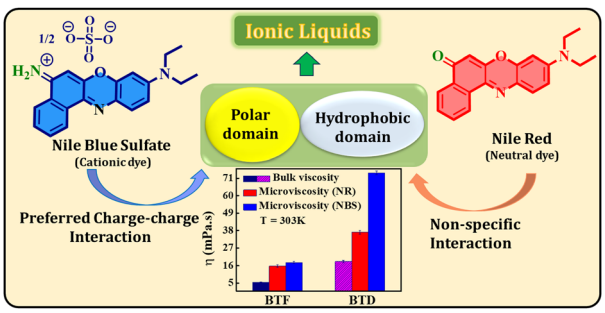
13335



Investigating the enhancement of lung cancer sensing: the effect of edge halogenation in armchair stanene nanoribbons

Maedeh Mashhadbani and Edris Faizabadi*

13350



Probing the heterogeneity of molecular level organization of ionic liquids: a comparative study using neutral Nile red and cationic Nile blue sulfate as fluorescent probes for butyrolactam-based protic ionic liquids

Bignya Rani Dash, Ramesh L. Gardas* and Ashok Kumar Mishra*

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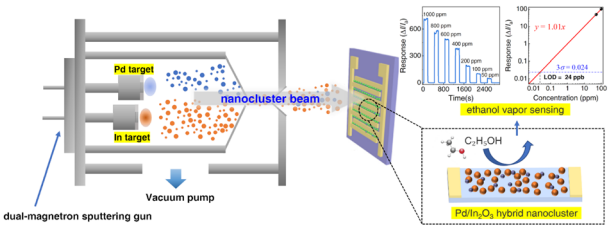
13364

Development of Pd/In_2O_3 hybrid nanoclusters to optimize ethanol vapor sensing

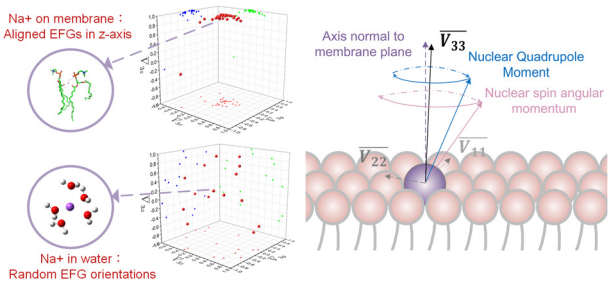
Bo Xie, Jian Sun, Aoxue Zhang, Haoyu Qian, Xibing Mao, Yingzhu Li, Wenjing Yan, Changjiang Zhou, Hui-Min Wen, Shengjie Xia, Min Han, Paolo Milani and Peng Mao*



13374

Nuclear spin alignment of sodium ions *via* electric field gradients in phospholipid membranes

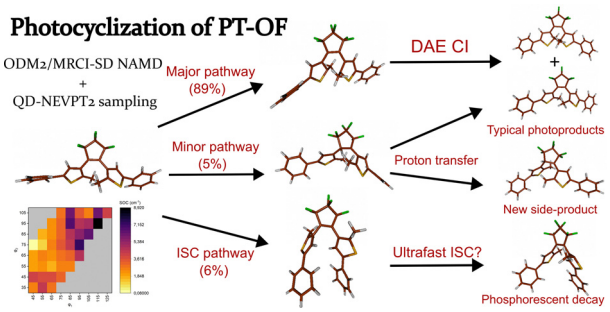
Yu Zheng and Quansheng Ren*



13383

New insights into the photocyclization reaction of a popular diarylethene switch: a nonadiabatic molecular dynamics study

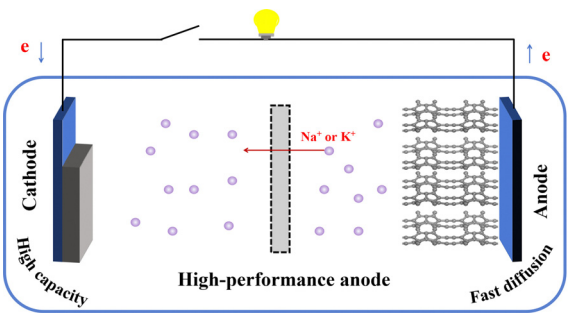
Mikołaj Martyka and Joanna Jankowska*



13395

Two-dimensional monolayer $C_{5\text{-}10\text{-}16}$: a metallic carbon allotrope as an anode material for high-performance sodium/potassium-ion batteries

Wen-Chun Wang, Ya-Qun Dai, Tian-Le Zhao, Xiao-Juan Ye,* Xiao-Hong Zheng, Ran Jia and Chun-Sheng Liu*



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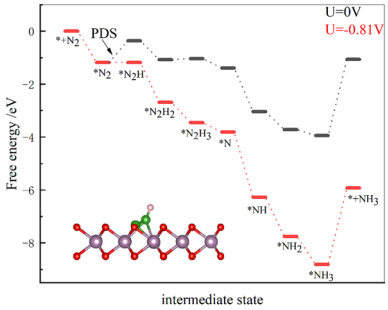
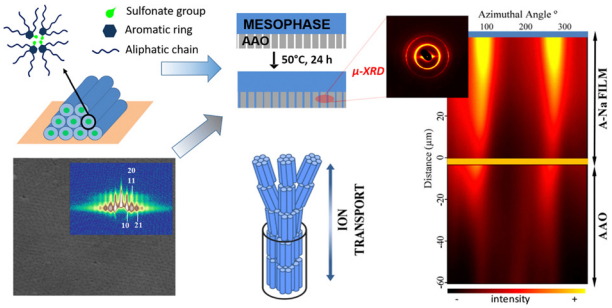


Theoretical study of the nitrogen reduction reaction catalyzed by a B-doped MoO_2 six-membered ring

Shaona Chen, Demiao Fang, Zhangyu Zhou, Zhongxu Dai* and Jinjin Shi*

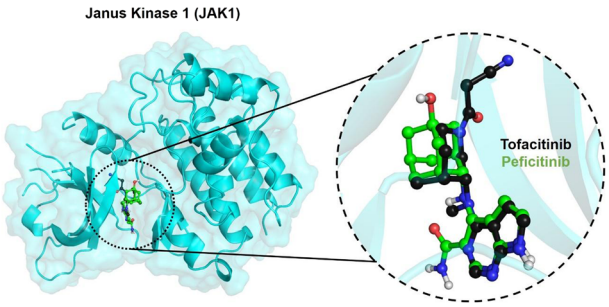
13412



Homeotropic orientation of an ion-channel forming mesophase induced by nanotemplate wetting

Jaime J. Hernandez,* Denis V. Anokhin, Martin Rosenthal, Xiaomin Zhu and Dimitri A. Ivanov*

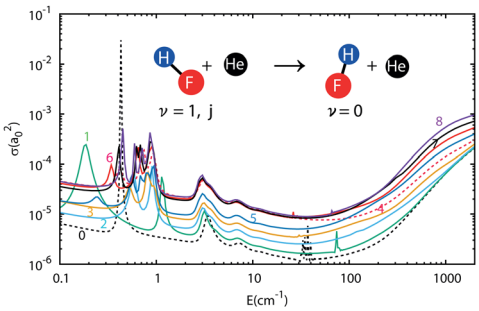
13420



Tofacitinib and peficitinib inhibitors of Janus kinase for autoimmune disease treatment: a quantum biochemistry approach

Jackson L. Amaral,* Naiara C. Lucredi, Victor L. B. França, Samuel J. M. Santos, Francisco F. Maia Jr, Pablo A. Morais, Pedro F. N. Souza, Jurandir F. Comar and Valder N. Freire

13432



Quantum study of the rovibrational relaxation of HF by collision with ^{4}He on a new potential energy surface

Otoniel Denis-Alpizar,* Alexandre Zanchet* and Thierry Stoecklin*

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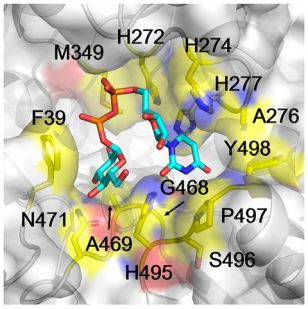
13441

A kinetic model reveals the critical gating motifs for donor-substrate loading into *Actinobacillus pleuropneumoniae* *N*-glycosyltransferase

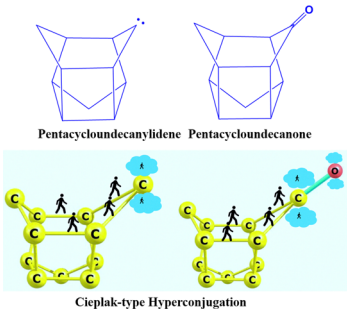
Zhiqiang Hao, Qiang Guo, Wenjie Peng* and Lin-Tai Da*



13452

Pentacycloundecanylidene and pentacycloundecanone – hyperconjugatively stabilized carbene and ketone

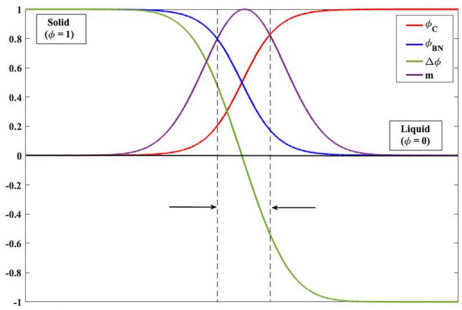
Jishnu Sai Gopinath and Pattiyil Parameswaran*



13463

Phase-field crystal modeling of graphene/hexagonal boron nitride interfaces

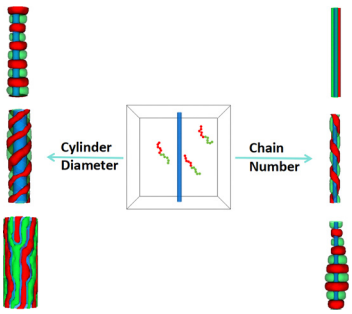
Shrikant S. Channe



13480

The mechanism underlying the transitions between stripes, helices, and stacked toroids in the cylindrical shell formed by AB diblock copolymers on a long nanocylinder

Hajinuer Bahetihan, Liangjun Ma and Weixin Kong*



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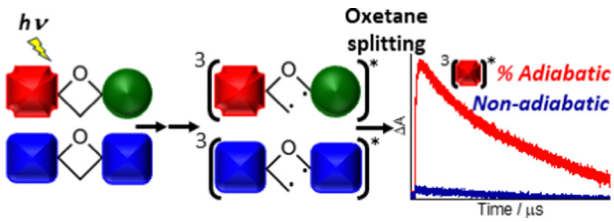
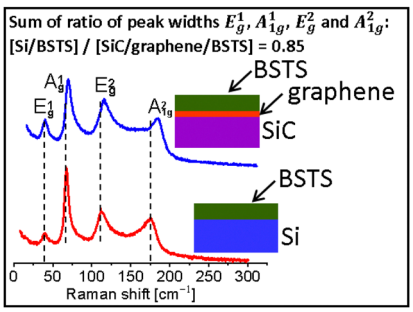


Photolytic splitting of homodimeric quinone-derived oxetanes studied by ultrafast transient absorption spectroscopy and quantum chemistry

Alejandro Blasco-Brusola, Lorena Tamarit, Miriam Navarrete-Miguel, Daniel Roca-Sanjuán, Miguel A. Miranda* and Ignacio Vayá*

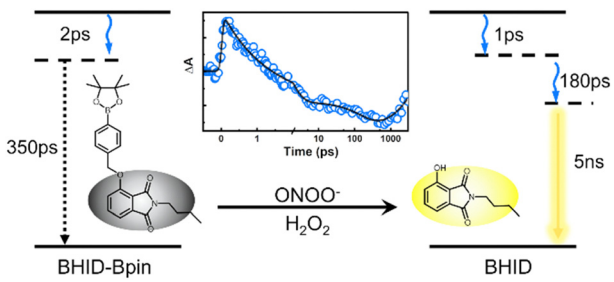
13497



Raman scattering spectroscopy of MBE grown thin film topological insulator $Bi_{2-x}Sb_xTe_{3-y}Se_y$

N. Kumar,* N. V. Surovtsev, P. A. Yunin, D. V. Ishchenko, I. A. Milekhin, S. P. Lebedev, A. A. Lebedev and O. E. Tereshchenko

13506



Excited-state dynamics of 4-hydroxyisoindoline-1,3-dione and its derivative as fluorescent probes

Li Zhao, Simin Jiang, Yanmei He, Luling Wu,* Tony D. James and Junsheng Chen*

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