

## IN THIS ISSUE

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### Cover

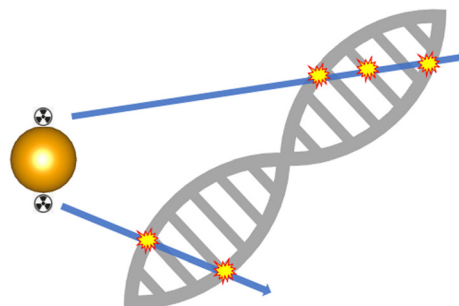
See Lai-Sheng Wang *et al.*,  
pp. 12928–12938.  
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*Phys. Chem. Chem. Phys.*,  
2024, 26, 12928.

## TUTORIAL REVIEW

12915

### <sup>211</sup>At on gold nanoparticles for targeted radionuclide therapy application

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

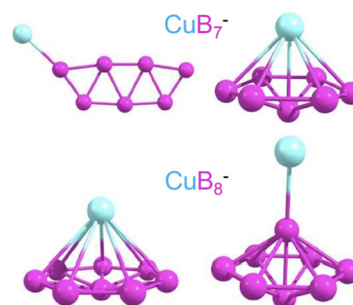


## RESEARCH PAPERS

12928

### Searching for stable copper borozene complexes in CuB<sub>7</sub><sup>−</sup> and CuB<sub>8</sub><sup>−</sup>

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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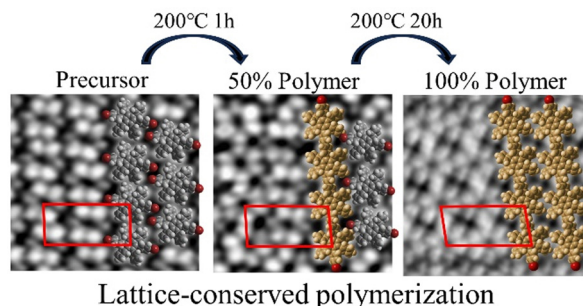


## RESEARCH PAPERS

12939

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

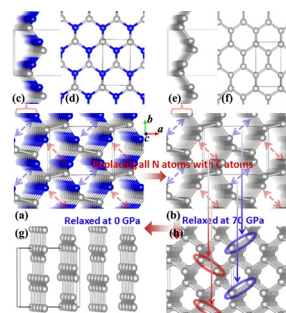
Hiroaki Ooe and Takashi Yokoyama\*



12947

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

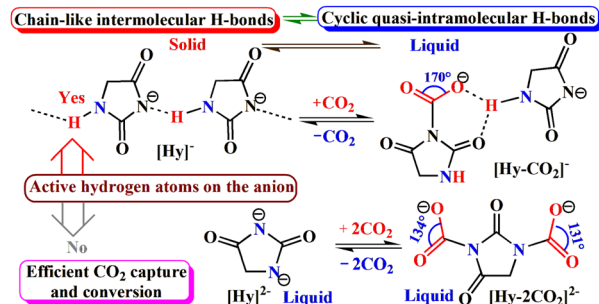
Haiping Wu,\* Yunhao Zheng, Erjun Kan and Yan Qian\*



12957

### Does the active hydrogen atom in the hydantoin anion affect the physical properties, CO<sub>2</sub> capture and conversion of ionic liquids?

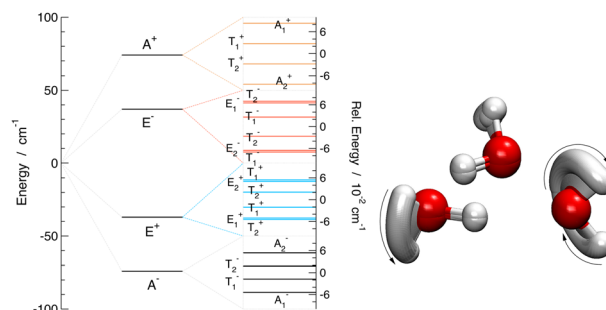
Tingting Chen, Zhongyuan Sun, Yujun Guo and Yingjie Xu\*



12965

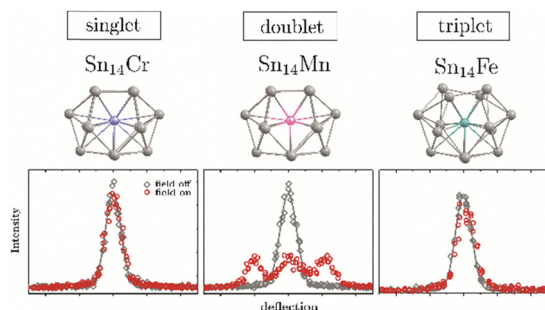
### Tunneling splittings in the vibrationally excited states of water trimer

Mihael Eraković and Marko T. Cvitaš\*



## RESEARCH PAPERS

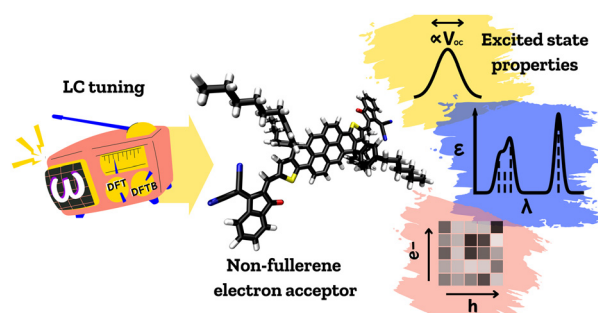
12982



**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

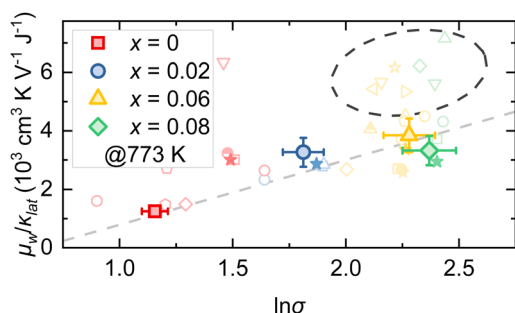
12993



**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

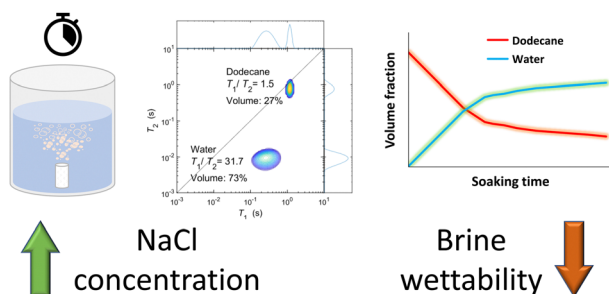
13006



**Thermoelectric properties of Bi<sub>1-x</sub>Pb<sub>x</sub>Cu<sub>1-x</sub>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\*

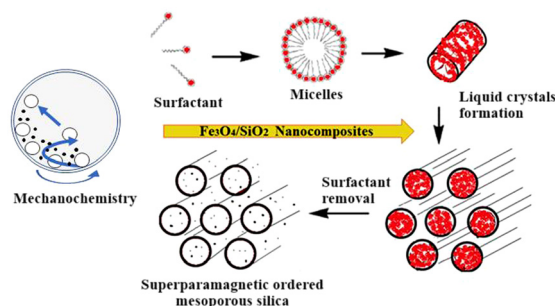


## RESEARCH PAPERS

13020

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

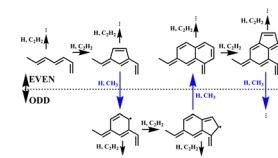
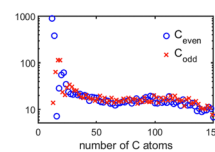
Alessandra Scano,\* Edmond Magner, Martina Pilloni, Luciano Atzori, Marzia Fantauzzi, Sawssen Slimani, Davide Peddis, Gonzalo Garcia Fuentes and Guido Ennas



13034

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

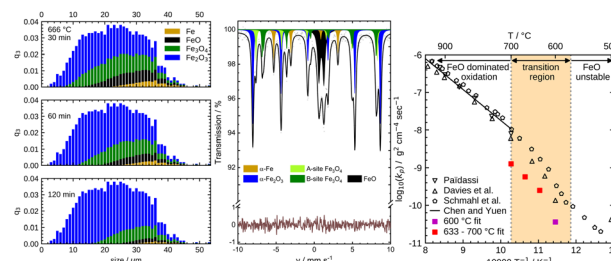
Michael Frenklach,\* Ahren W. Jasper and Alexander M. Mebel\*



13049

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

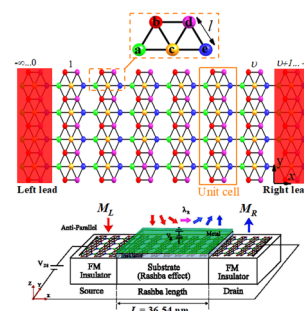
Jonas Spielmann, Daniel Braig, Antonia Streck, Tobias Gustmann, Carola Kuhn, Felix Reinauer, Alexandr Kurnosov, Oliver Leubner, Vasily Potapkin, Christian Hasse, Olaf Deutschmann, Bastian J. M. Etzold, Arne Scholtissek\* and Ulrike I. Kramm\*



13061

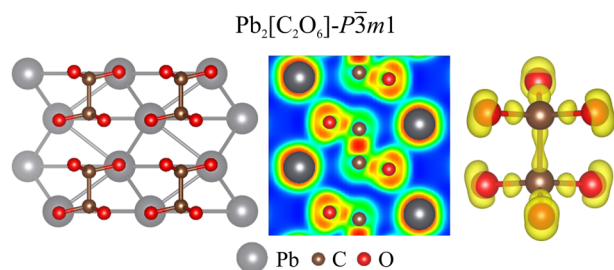
# Ultrafast switching in spin field-effect transistors based on borophene nanoribbons

Farzaneh Ghasemzadeh, Mohsen Farokhnezhad\* and Mahdi Esmaeilzadeh\*



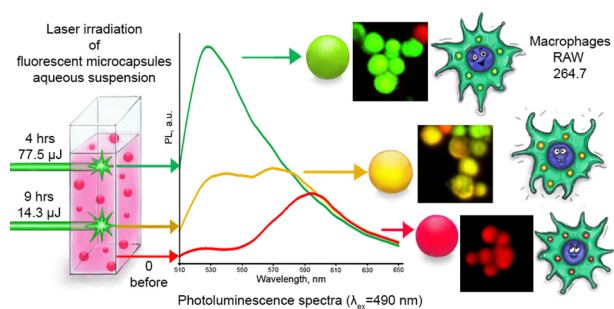
## RESEARCH PAPERS

13070

 **$\text{Pb}_2[\text{C}_2\text{O}_6] \cdot P\bar{3}m1$ : new insights into the high-pressure behavior of carbonates**

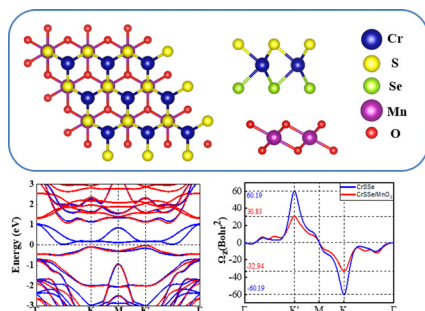
Maksim V. Banaev,\* Dinara N. Sagatova,\*  
Nursultan E. Sagatov and Pavel N. Gavryushkin

13078

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

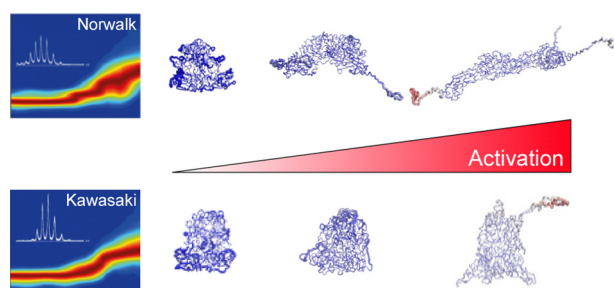
Polina A. Demina,\* Oleg V. Grishin, Sergey N. Malakhov,  
Olesya I. Timaeva, Elizaveta S. Kulikova,  
Timofey E. Pylaev, Mariia S. Saveleva and  
Irina Yu. Goryacheva

13087

**Enhancement and modulation of valley polarization in Janus  $\text{CrSSe}$  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 Coleman and Erik G. Marklund\*

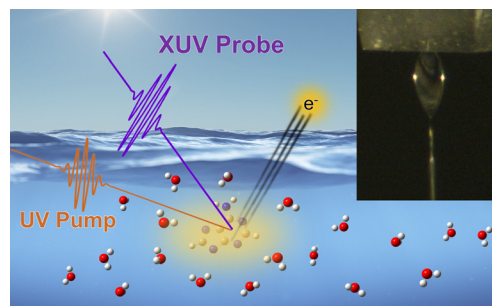


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13106

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

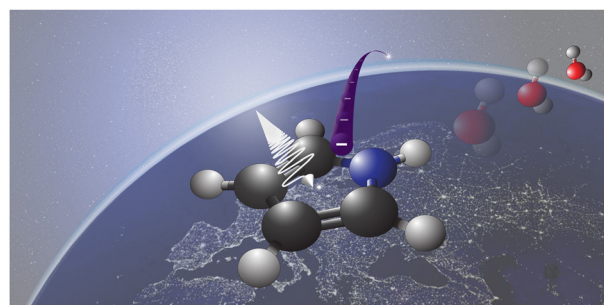
Masafumi Koga, Do Hyung Kang, Zachary N. Heim, Philipp Meyer, Blake A. Erickson, Neal Haldar, Negar Baradaran, Martina Havenith and Daniel M. Neumark\*



13118

**Water is a radiation protection agent for ionised pyrrole**

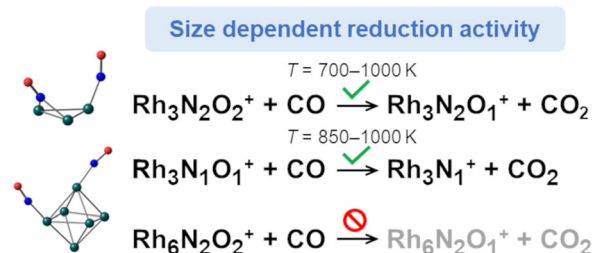
Melby Johny, Constant A. Schouder, Ahmed Al-Refaie, Lanhai He, Joss Wiese, Henrik Stapelfeldt, Sebastian Trippel\* and Jochen Küpper



13131

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

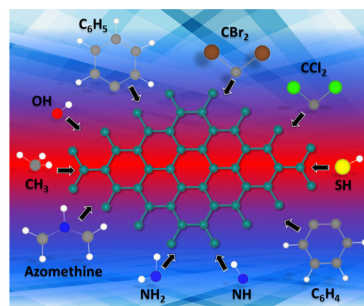
Ken Miyajima, Toshiaki Nagata, Fumitaka Mafuné,\* Tomoya Ichino, Satoshi Maeda, Taizo Yoshinaga, Masahide Miura and Takahiro Hayashi



13140

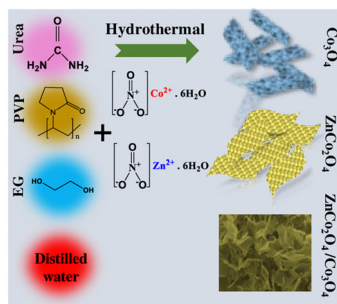
**Covalent functionalization of germanene employing computational simulations**

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



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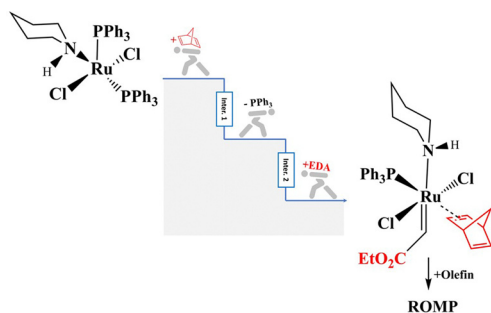
13152



### Synergistic effect between $\text{ZnCo}_2\text{O}_4$ and $\text{Co}_3\text{O}_4$ induces superior electrochemical performance as anodes for lithium-ion batteries

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

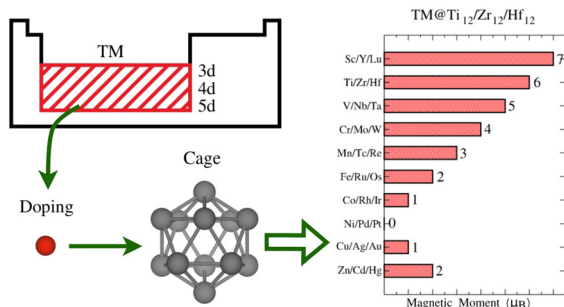
13164



### Structural and thermodynamic insights into the coordination preference of norbornadiene with the initiator complex $[\text{RuCl}_2(\text{PPh}_3)_2(\text{piperidine})]$ 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\*

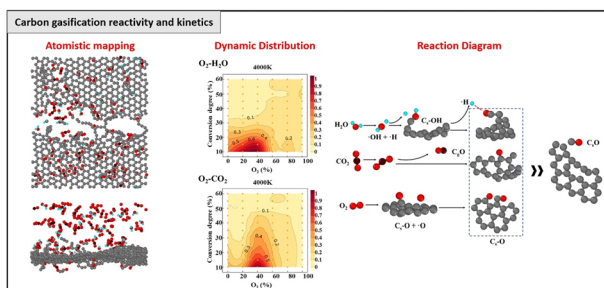
13172



### 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 $\text{O}_2/\text{H}_2\text{O}$ and $\text{O}_2/\text{CO}_2$ on gasification reactivity and kinetics

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

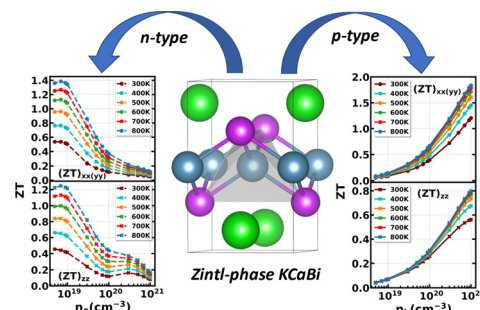


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13198

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

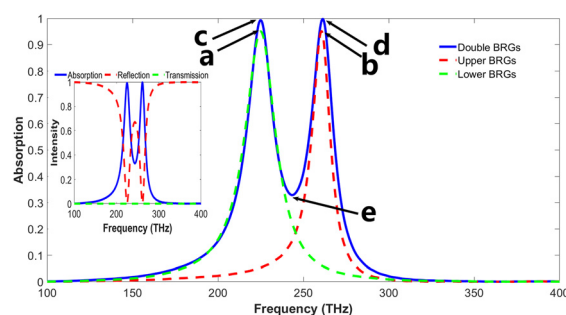
Sampad Mandal, Atish Ghosh and Pranab Sarkar\*



13209

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

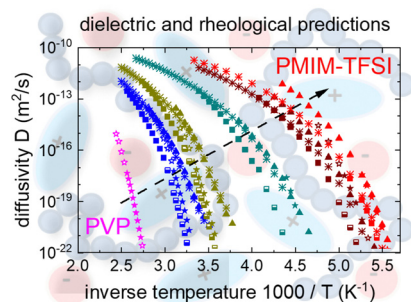
Yizhao Pan, Yuchang Li, Fang Chen,\* Wenxing Yang and Zao Yi



13219

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

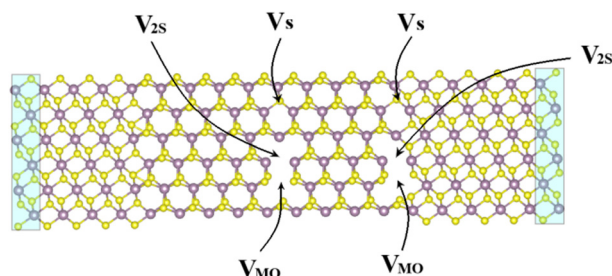
Lara Röwekamp, Kevin Moch,\* Merve Seren, Philipp Münzner, Roland Böhmer and Catalin Gainaru



13230

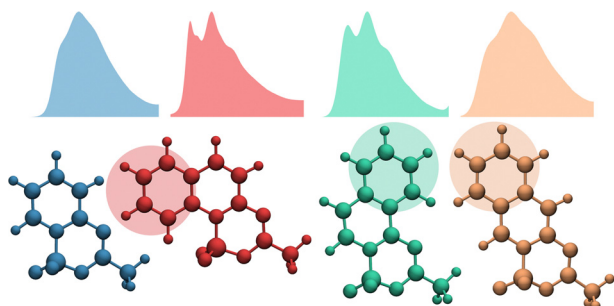
## Effect of point defects on the band alignment and transport properties of 1T-MoS<sub>2</sub>/2H-MoS<sub>2</sub>/1T-MoS<sub>2</sub> heterojunctions

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



## RESEARCH PAPERS

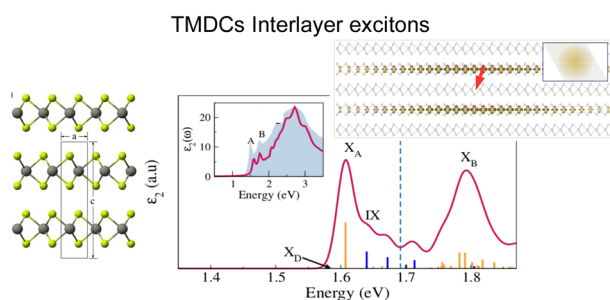
13239



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

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

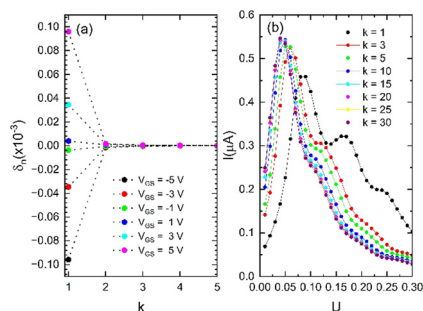
13251



### Optical spectra and exciton radiative lifetimes in bulk transition metal dichalcogenides

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

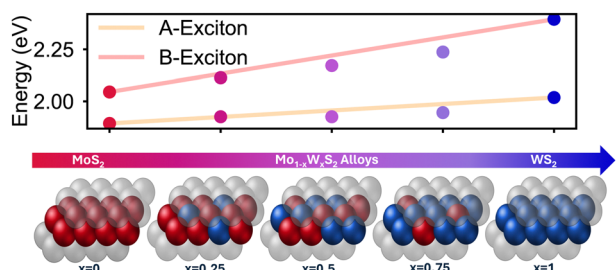
13261



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

Shih-Jye Sun,\* Miroslav Menšík and Petr Toman

13271



### Colloidal 2D Mo<sub>1-x</sub>W<sub>x</sub>S<sub>2</sub> 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\*

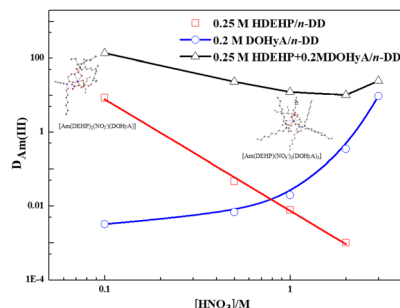


## RESEARCH PAPERS

13279

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

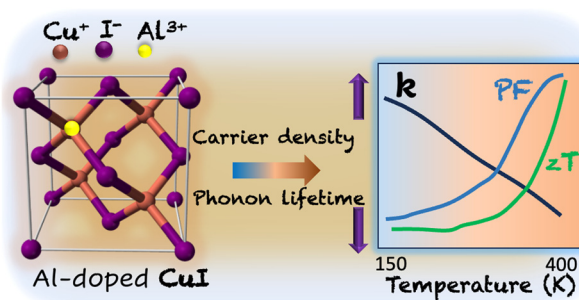
K. Rama Swami,\* N. Parvathy, Abigail Jennifer G, Ramesh L. Gardas and Elumalai Varathan\*



13287

### Probing the thermoelectric properties of aluminium-doped copper iodide

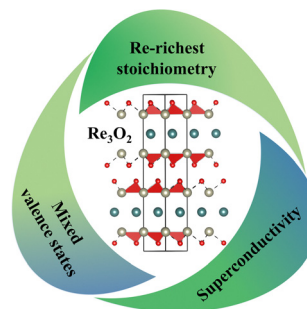
Tatavarthi Veera Venkata Ramana,\* Manjusha Battabyal,\* Santosh Kumar, Dillip K. Satapathy\* and Ravi Kumar\*



13300

### Metallic $\text{Re}_3\text{O}_2$ with mixed-valence states

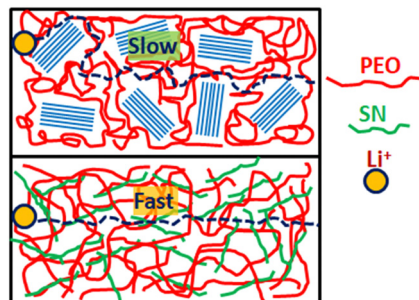
Wenjing Li, Fei Li,\* Xiaohua Zhang, Jinhui Wu and Guochun Yang\*



13306

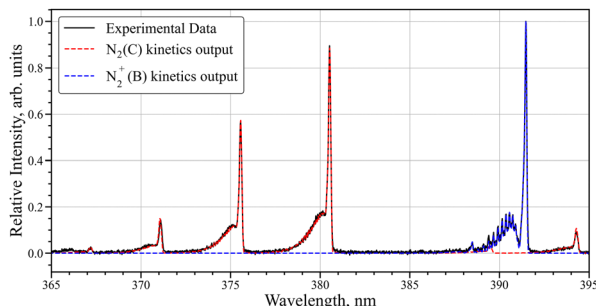
### Decoupling of ion-transport from polymer segmental relaxation and higher ionic-conductivity in poly(ethylene oxide)/succinonitrile composite-based electrolytes having low lithium salt doping

J. Mor and S. K. Sharma\*



## RESEARCH PAPERS

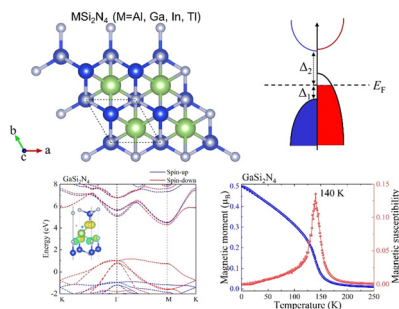
13316



## Spectral analysis and kinetic modeling of radioluminescence in air and nitrogen

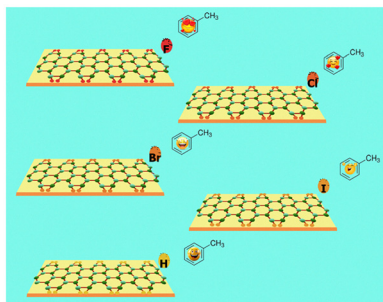
E. R. Jans,\* T. Casey, G. J. Marshall, C. M. Murzyn, S. S. Harilal, B. S. McDonald and R. K. Harrison

13327

Two-dimensional half-metals  $\text{MSi}_2\text{N}_4$  ( $M = \text{Al}, \text{Ga}, \text{In}, \text{Tl}$ ) with intrinsic p-type ferromagnetism and ultrawide bandgaps

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

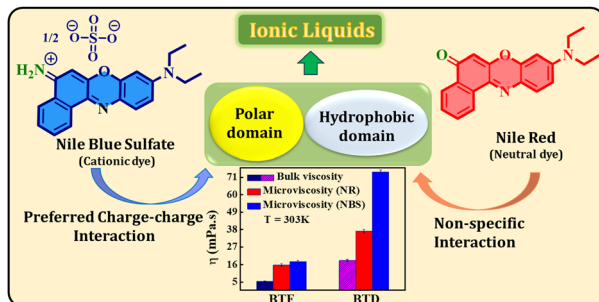
13335



## 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\*

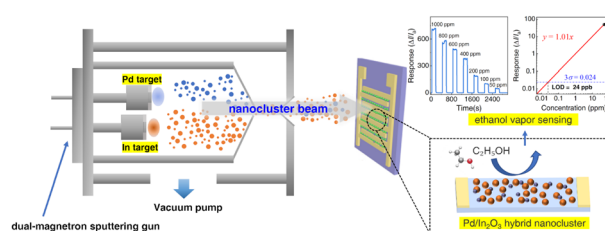


## RESEARCH PAPERS

13364

Development of Pd/In<sub>2</sub>O<sub>3</sub> hybrid nanoclusters to optimize ethanol vapor sensing

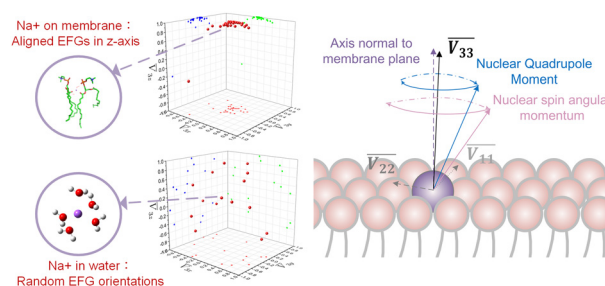
Bo Xie, Jian Sun, Aoxue Zhang, Haoyu Qian, Xibing Mao, Yingzhu Li, Wenjing Yan, Changjiang Zhou, Hui-Min Wen, Shengjie Xia, Min Han, Paolo Milani and Peng Mao\*



13374

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

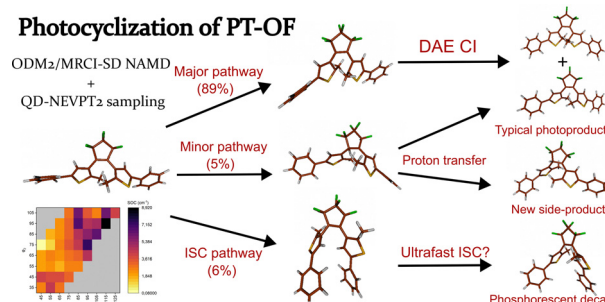
Yu Zheng and Quansheng Ren\*



13383

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

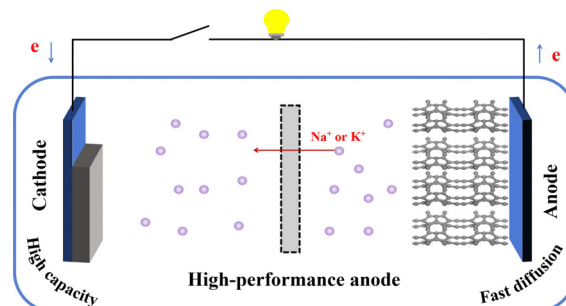
Mikotaj Martyka and Joanna Jankowska\*



13395

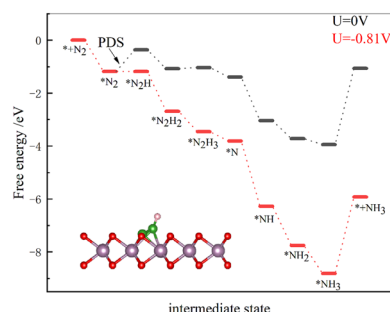
Two-dimensional monolayer C<sub>5-10-16</sub>: a metallic carbon allotrope as an anode material for high-performance sodium/potassium-ion batteries

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



## RESEARCH PAPERS

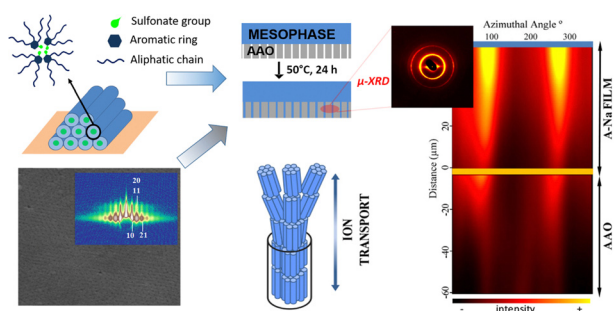
13405



### Theoretical study of the nitrogen reduction reaction catalyzed by a B-doped MoO<sub>2</sub> six-membered ring

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

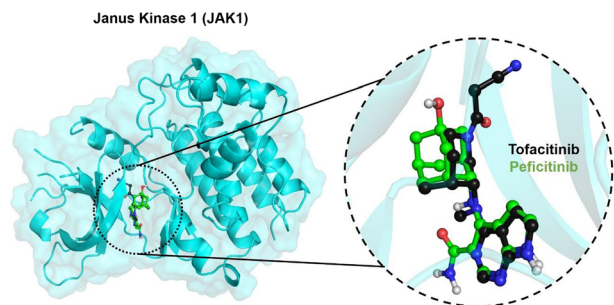
13412



### 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\*

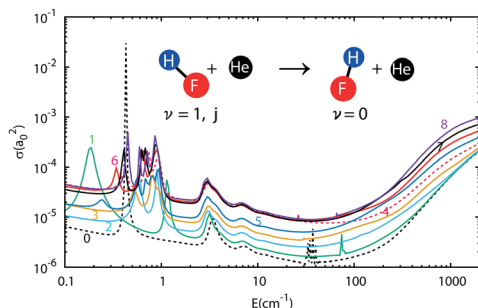
13420



### 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. Moraes, Pedro F. N. Souza, Jurandir F. Comar and Valder N. Freire

13432



### Quantum study of the rovibrational relaxation of HF by collision with <sup>4</sup>He on a new potential energy surface

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

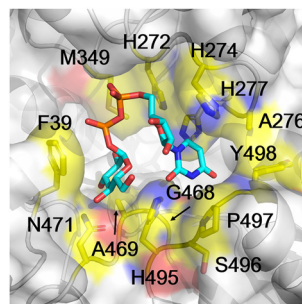


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13441

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

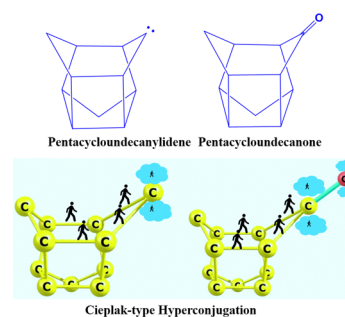
Zhiqiang Hao, Qiang Guo, Wenjie Peng\* and Lin-Tai Da\*



13452

### Pentacycloundecanylidene and pentacycloundecanone – hyperconjugatively stabilized carbene and ketone

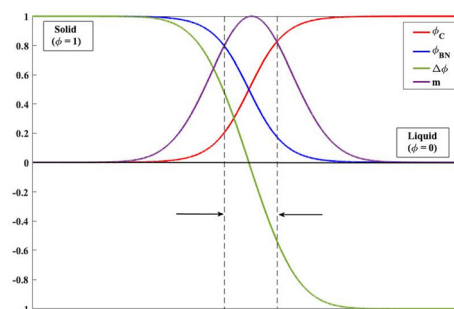
Jishnu Sai Gopinath and Pattiyil Parameswaran\*



13463

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

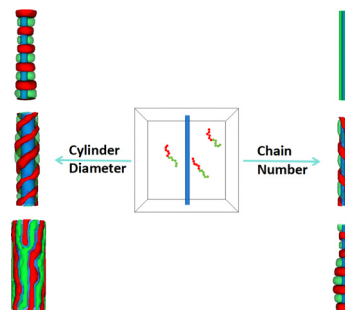
Shrikant S. Channe



13480

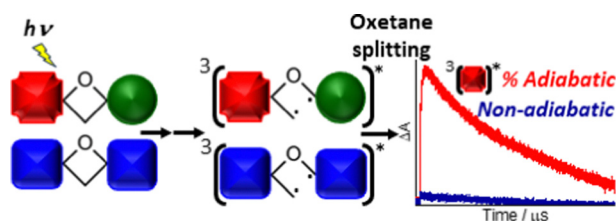
### The mechanism underlying the transitions between stripes, helices, and stacked toroids in the cylindrical shell formed by AB diblock copolymers on a long nanocylinder

Hajinuer Bahetihan, Liangjun Ma and Weixin Kong\*



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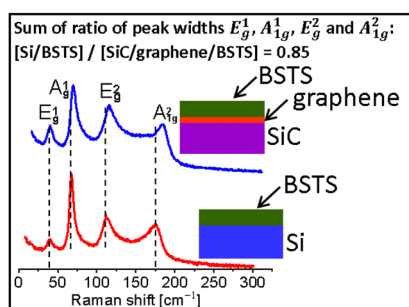
13489



### 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\*

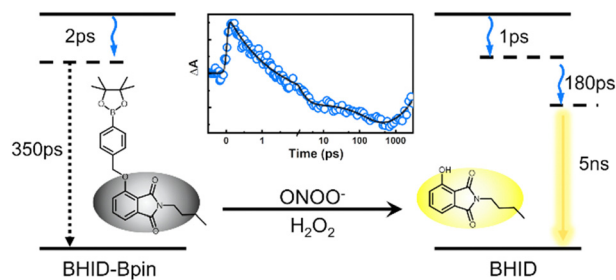
13497



### Raman scattering spectroscopy of MBE grown thin film topological insulator $\text{Bi}_{2-x}\text{Sb}_x\text{Te}_{3-y}\text{Se}_y$

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-hydroxyisindoline-1,3-dione and its derivative as fluorescent probes

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

