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#### Inside cover

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*Phys. Chem. Chem. Phys.*,  
2024, **26**, 16955.

### EDITORIAL

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#### Physical chemistry of the energy transition

Robert Schlögl, Alec M. Wodtke, Timo Jacob and Swetlana Schauermann



Timo Jacob (Ulm  
University)



Swetlana Schauermann (Kiel University)

#### Bunsen-Tagung 2023: Physical Chemistry of the Energy Transition



Robert Schlögl (Fritz Haber  
Institute of the Max Planck  
Society)



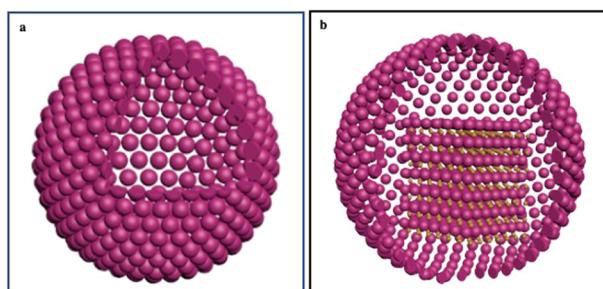
Alec Wodtke (Georg-August  
University & Department of  
Dynamics at Surfaces, Max-Planck-  
Institute for Multidisciplinary  
Sciences)

### PERSPECTIVE

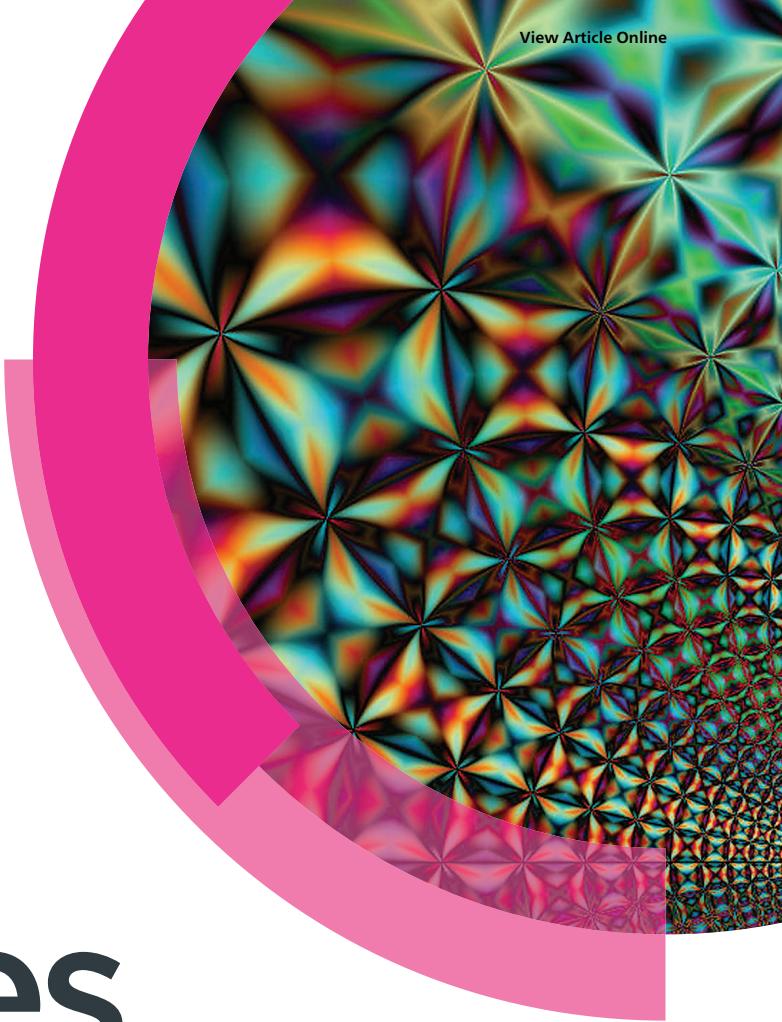
16931

#### “Nano-egg” superstructures of hydrophobic nanocrystals dispersed in water

M. P. Pilani



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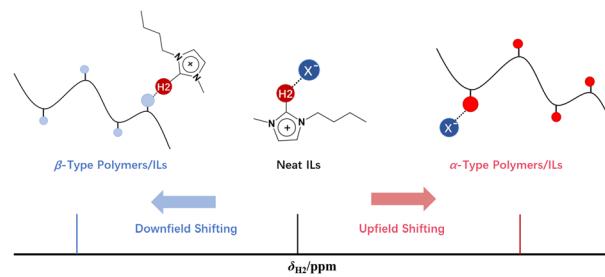
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## COMMUNICATION

16942

**Polymer solubility mechanism in ionic liquids:  
<sup>1</sup>H-NMR spectra and two-parameter hydrogen  
bonding analysis**

Ming-Xuan Du,\* Ya-Fei Yuan, Jin-Ming Zhang,  
Jia-Jian Liu and Chen-Yang Liu\*

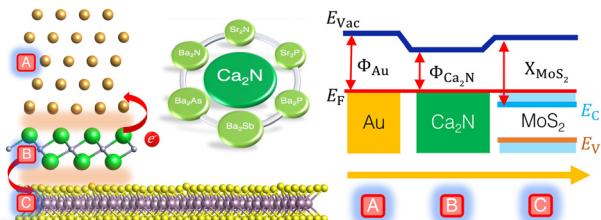


## RESEARCH PAPERS

16947

**Designing barrier-free metal/MoS<sub>2</sub> contacts  
through electrene insertion**

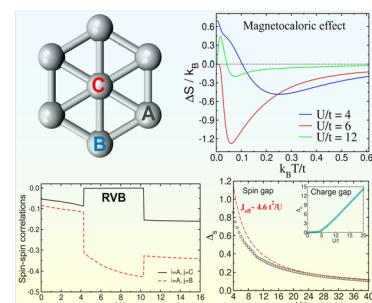
Mohammad Rafiee Diznab, Adrian F. Rumson,  
Jesse Maassen\* and Erin R. Johnson\*



16955

**Thermodynamics of resonating-valence-bond  
states toward the understanding of quantum  
spin liquid phenomena**

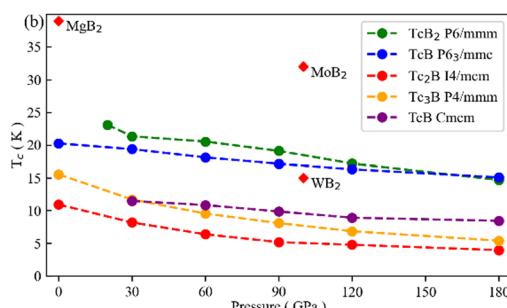
Florentino López-Urías,\* Alberto Rubio-Ponce,  
Emilio Muñoz-Sandoval and Francisco Sánchez-Ochoa



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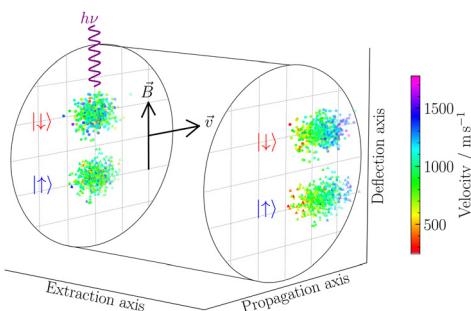
**Discovery of superconductivity in technetium  
borides at moderate pressures**

Xiangru Tao, Aiqin Yang, Yundi Quan, Biao Wan,  
Shuxiang Yang\* and Peng Zhang\*



## RESEARCH PAPERS

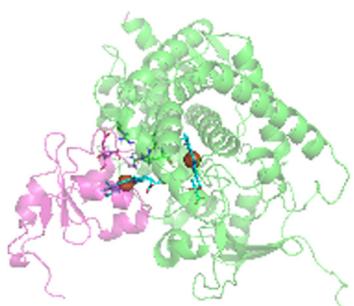
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## Out-of-focus spatial map imaging of magnetically deflected sodium ammonia clusters

D. P. Borgeaud dit Avocat, H. Yang, A. Nitsche, J. Wenger, B. L. Yoder and R. Signorell\*

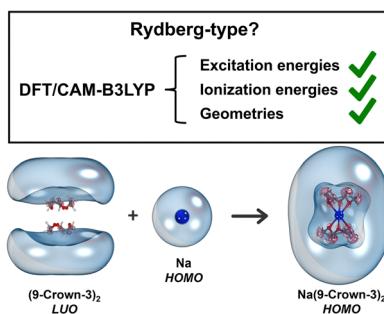
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## Tracking protein–protein interactions by NMR: conformational selection in human steroidogenic cytochrome P450 CYP17A1 induced by cytochrome *b*<sub>5</sub>

Alaina M. Richard, D. Fernando Estrada, Liam Flynn, Susan Sondej Pochapsky, Emily E. Scott and Thomas C. Pochapsky\*

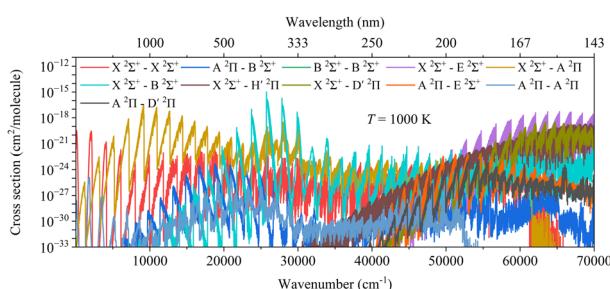
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## Electronic structure analysis and DFT benchmarking of Rydberg-type alkali-metal-crown ether, -cryptand, and -adamanzane complexes

Isuru R. Ariyarathna

16998



## An *ab initio* diabatic study of rovibronic spectra of CN

Shuai Zhang, Zhi Qin and Linhua Liu\*

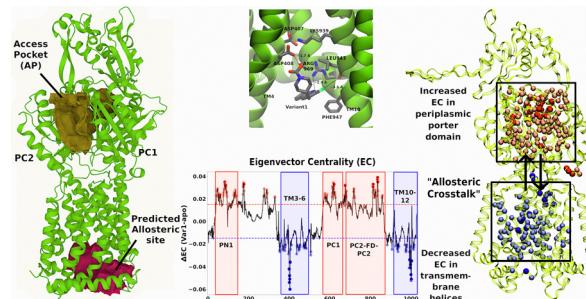


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**Exploring transmembrane allostericity in the MexB: DB08385 variant as a promising inhibitor-like candidate against *Pseudomonas aeruginosa* antibiotic resistance: a computational study**

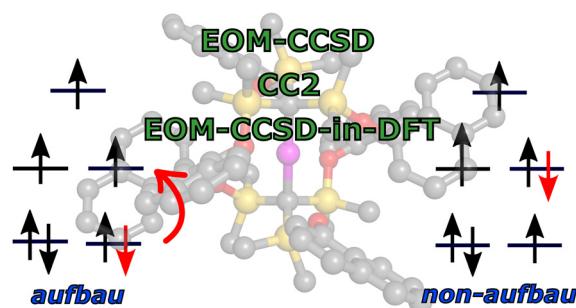
Abhishek Bera, Shreya Mukherjee and Niladri Patra\*



17028

**Coupled-cluster treatment of complex open-shell systems: the case of single-molecule magnets**

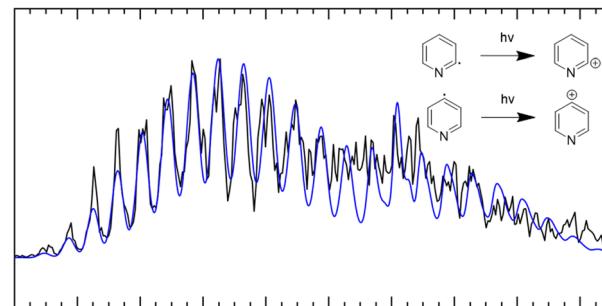
Maristella Alessio,\* Garrette Pauley Paran, Cansu Utku, Andreas Grüneis and Thomas-C. Jagau



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**Photoelectron spectrum of the pyridyl radical**

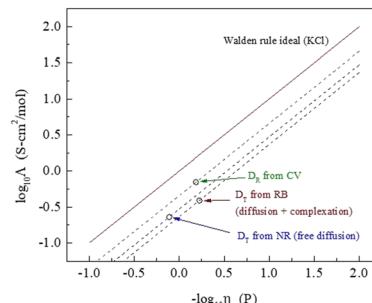
Emil Karaev, Marius Gerlach, Katharina Theil, Gustavo A. Garcia, Christian Alcaraz, Jean-Christophe Loison and Ingo Fischer\*



17048

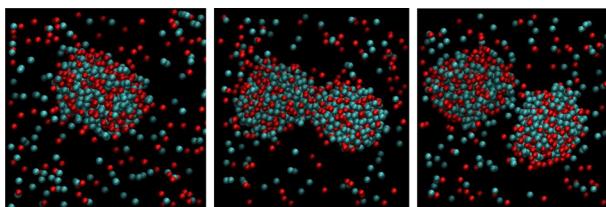
**Evaluating the contributions to conductivity in room temperature ionic liquids**

Emily D. Simonis and G. J. Blanchard\*



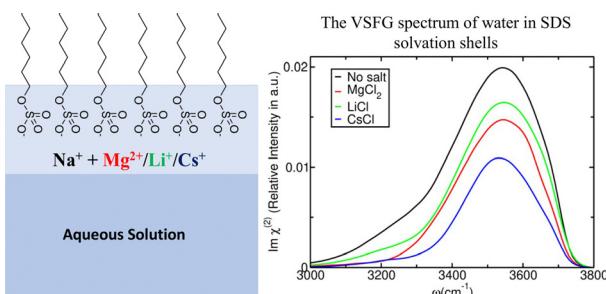
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**Secondary nucleation in symmetric binary SALR mixtures**

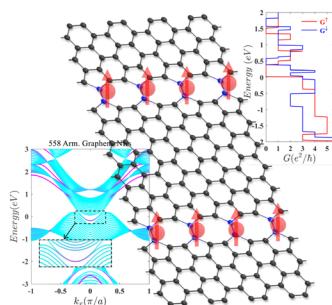
Jiazheng Tan and Martin B. Sweatman\*

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**Effect of counterions on the structure and dynamics of water near a negatively charged surfactant: a theoretical vibrational sum frequency generation study**

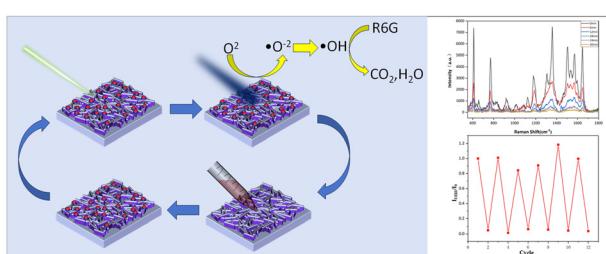
Ravi Malik, Shinji Saito\* and Amalendu Chandra\*

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**Topological phases, local magnetic moments, and spin polarization triggered by C<sub>558</sub>-line defects in armchair graphene nanoribbons**

Ning-Jing Yang, Wen-Ti Guo, Hai Yang, Zhigao Huang and Jian-Min Zhang\*

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**Ag/ZnO microcavities with high sensitivity and self-cleaning properties for fast repetitive SERS detection**

Jiale Zheng, Dongliang Liu, Xilong Liu, Zekai Wang, Junfeng Li, Xinxin Wang, Jun Wang, Qiang Fu, Yanqiang Cao, Liyong Jiang and Yikai Chen\*

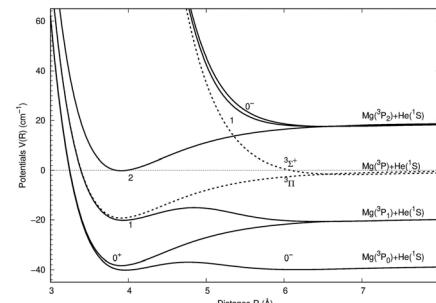


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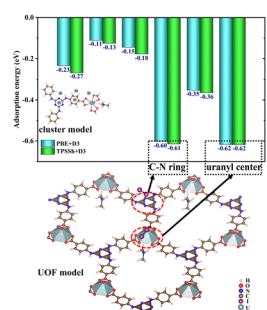
**Theoretical study of the spin-orbit coupled molecular states of the Mg–He dimer**

K. Alioua



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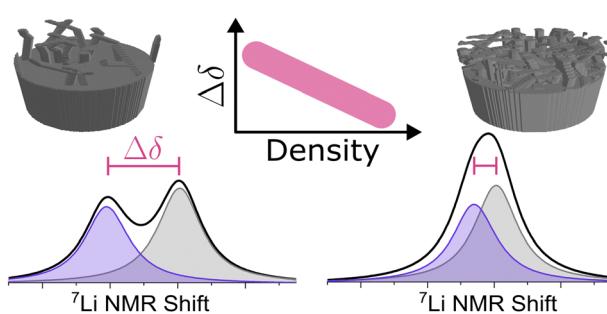
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### Iodine capture of a two-dimensional layered uranyl-organic framework: a combined DFT and AIMD study

Mingyang Shi, Kunyang Cheng, Xiujuan Cheng, Xuying Zhou, Gang Jiang and Jiguang Du\*

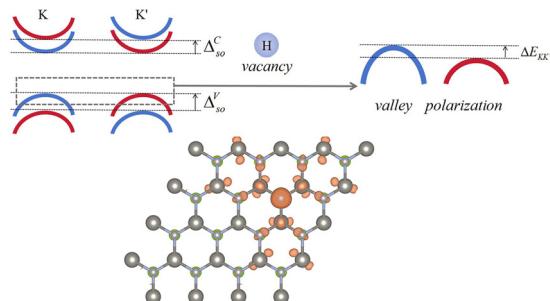
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### Morphology characterization of dendrites on lithium metal electrodes by NMR spectroscopy

Santiago Agustín Maldonado-Ochoa,\* Muriel Zampieri, Manuel Otero and Fabián Vaca Chávez\*

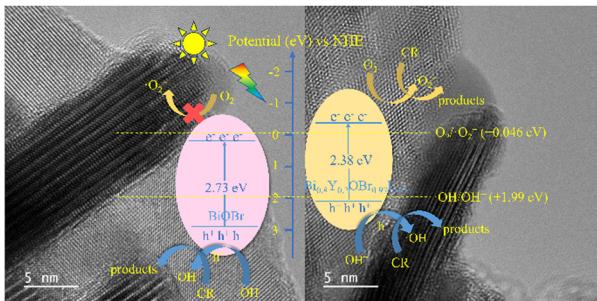
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Ziqi Wang, Xuening Han and Yan Liang\*

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Dongsheng Chen, Keqian Gong, Xiangyang Xu,\* Chenyu Huang and Pengtao Lei

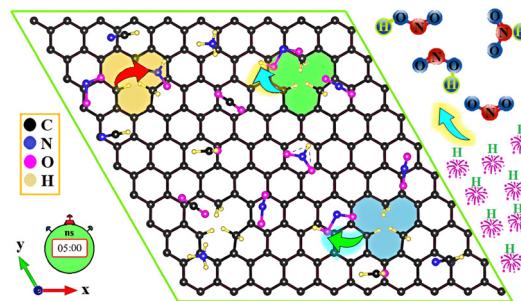


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**Disclosure of the nano-scale hydrogen dynamics on mono-vacancy graphene: a reactivity study with incoming gases**

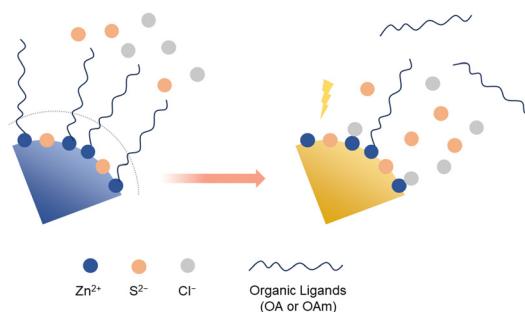
Nasim Hassani



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**ZnSeTe quantum dots modified with zinc chloride toward bright trap-state emission**

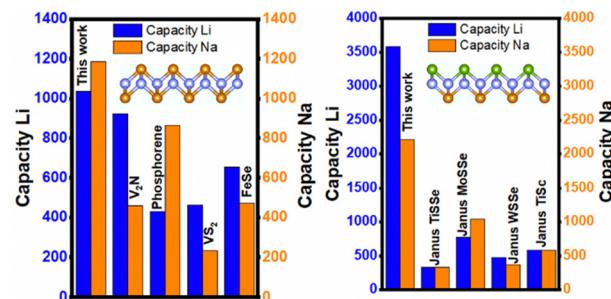
Zhe-Yong Chen, Xue Ren, Hui-Ling Hu, Meng Liu, Yi Liu and Feng-Lei Jiang\*



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**Metallic CoSb and Janus Co<sub>2</sub>AsSb monolayers as promising anode materials for metal-ion batteries**

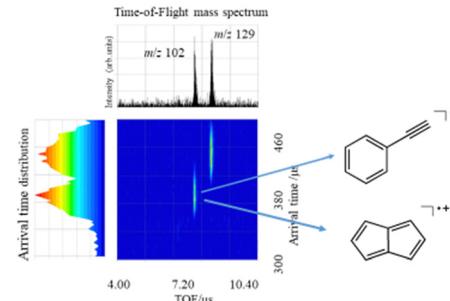
Dildar Ahmed, Nisar Muhammad and Z. J. Ding\*



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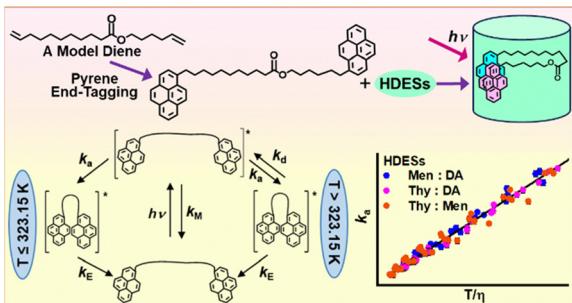
**Structural analysis of C<sub>8</sub>H<sub>6</sub><sup>•+</sup> fragment ion from quinoline using ion-mobility spectrometry/mass spectrometry**

Kenichi Iwamoto,\* Genki Inoue and Hiroshi Matsubara



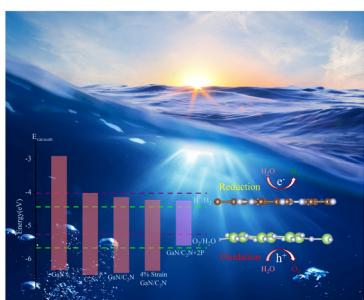
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**Assessing hydrophobic deep eutectic solvents for intramolecular excimer formation**

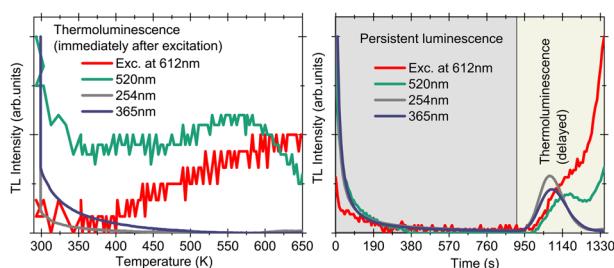
Shreya Juneja and Siddharth Pandey\*

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**Doping and strain modulation of the electronic, optical and photocatalytic properties of the GaN/C<sub>x</sub>N heterostructure**

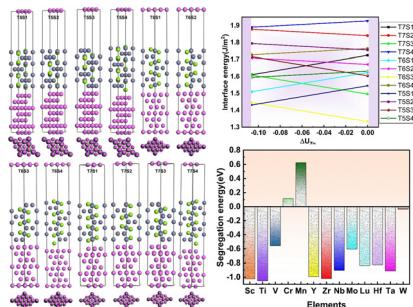
Fu Yin, Hui Wang,\* Zhengqin Zhao, LiJia Luo, Yongliang Tang, Yanbo Zhang and Qiang Xue

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**Delayed tunneling of charges to deep traps in a ZnO impurity containing Cr<sup>3+</sup> doped Zn<sub>2</sub>TiO<sub>4</sub> inverse spinel**

Ankit Sharma and Suchinder K. Sharma\*

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**The first-principles study of interfacial bonding strength and segregation behavior of alloyed elements at the  $\eta(\text{MgZn}_2)/\text{Al}$  interface**

Qing Gao, Guoyu Qiao, Weibing Wang, Yuxiang Ge, Junqiang Ren, Wei Li, Ping Yang, Xuefeng Lu\* and Jisen Qiao\*

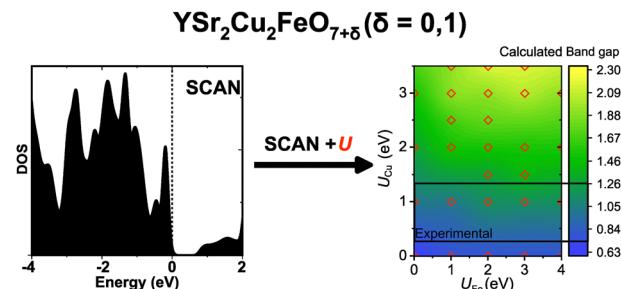


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**The SCAN+U method in the investigation of complex transition metal oxides: a case study on  $\text{YSr}_2\text{Cu}_2\text{FeO}_{7+\delta}$  ( $\delta = 0, 1$ )**

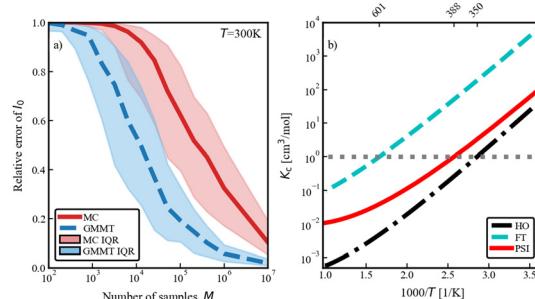
Marianela Gómez-Toledo and Elena M. Arroyo-de Dompablo\*



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**Importance sampling within configuration space integration for adsorbate thermophysical properties: a case study for  $\text{CH}_3/\text{Ni}(111)$**

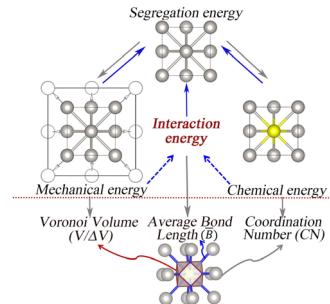
Katrín Blöndal, Kirk Badger, Khachik Sargsyan, David H. Bross, Branko Ruscic and C. Franklin Goldsmith\*



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**Preferential segregation of gold at the symmetrical tilt grain boundaries of platinum: an atomic-scale quantitative understanding**

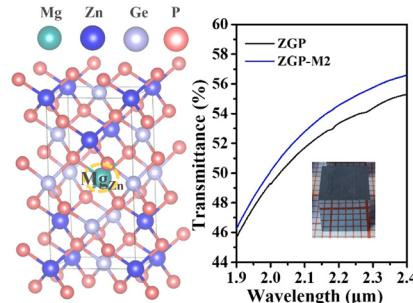
Xianxian Zhang, Jianfeng Tang,\* Xingming Zhang, Liang Wang, Dingwang Yuan, Huiqiu Deng and Lei Deng\*



17282

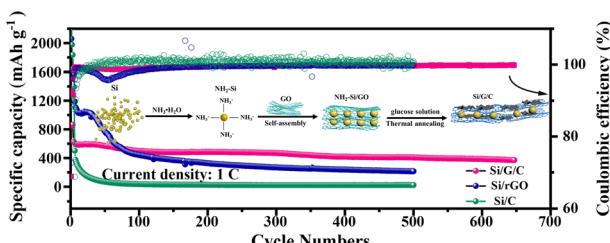
**Enhanced near-infrared optical transmission in zinc germanium phosphide crystals via precise magnesium doping**

Shichao Cheng, Xueyan Zhang, Xiangran Kong, Tao Liu, Jingdong Yan, Tetiana Prikhna, Yunfei Shang,\* Zuotao Lei\* and Chunhui Yang



## RESEARCH PAPERS

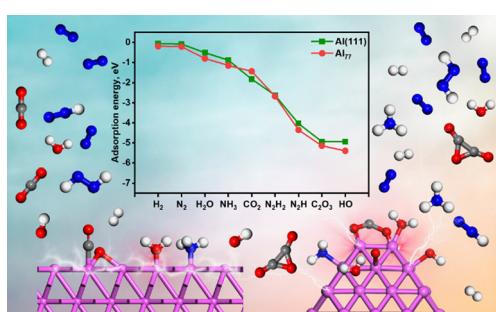
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### Carbon-coated silicon/graphite oxide composites as anode materials for highly stable lithium-ion batteries

Lujie Niu, Rui Zhang,\* Qiang Zhang, Dong Wang, Yanlei Bi, Guangwu Wen and Lu-Chang Qin

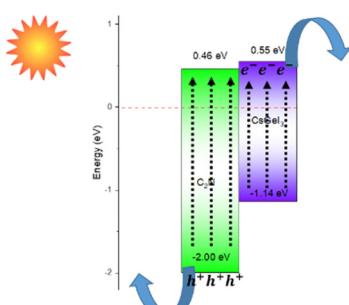
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### Adsorption mechanisms of decomposition species of CHON-containing explosives on aluminum surfaces

Kai Zhong and Chaoyang Zhang\*

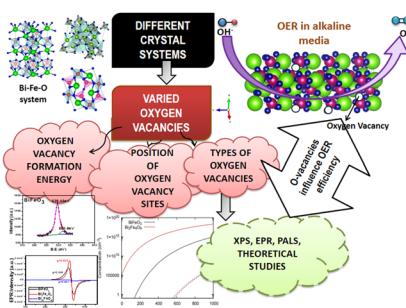
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### The lead-free perovskite-based heterojunction C<sub>2</sub>N/CsGel<sub>3</sub>: an exploration for superior visible-light absorption

Junli Chang,\* Yumeng Xie, Wenwu Shi, Jinguo Jiang, Hongyan Zhang and Guangzhao Wang\*

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### Electrocatalytic OER behavior of the Bi-Fe-O system: an understanding from the perspective of the presence of oxygen vacancies

Shaswati Jyoti, Aditi Vijay, Umberto Terranova, Santosh K Gupta, Kathi Sudarshan and Sonalika Vaidya\*

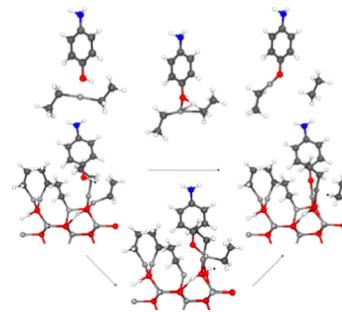


## RESEARCH PAPERS

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**Modelling the growth reaction pathways of zincone ALD/MLD hybrid thin films: a DFT study**

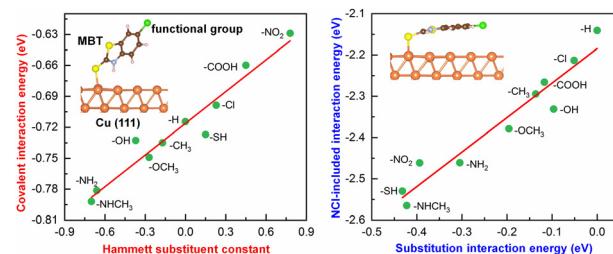
Mario Mäkinen,\* Timo Weckman and Kari Laasonen



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**Unravelling the effects of functional groups on the adsorption of 2-mercaptobenzothiazole on a copper surface: a DFT study**

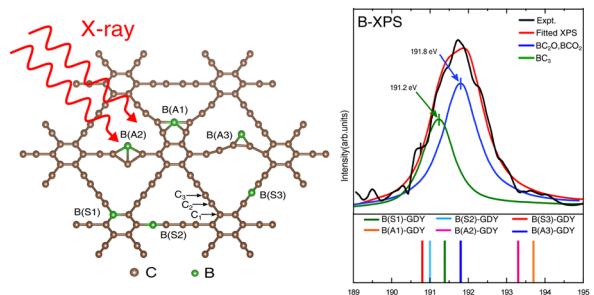
Thanh Hai Pham, Viorel Chihaiia and Do Ngoc Son\*



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**Structural identification of single boron-doped graphdiynes by computational XPS and NEXAFS spectroscopy**

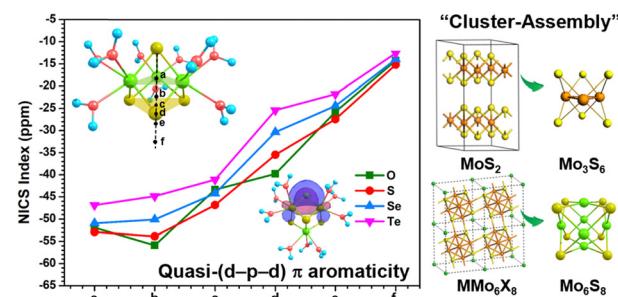
Hai-Bo Li, Jun-Rong Zhang,\* Xiu-Neng Song, Chuan-Kui Wang, Weijie Hua and Yong Ma\*



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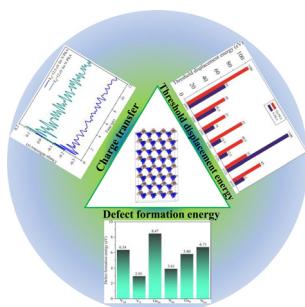
**Revisiting the quasi-aromaticity in polynuclear metal chalcogenide clusters and their derivative "cluster-assembly" crystalline structures**

Bochu Wang and Wan-Lu Li\*



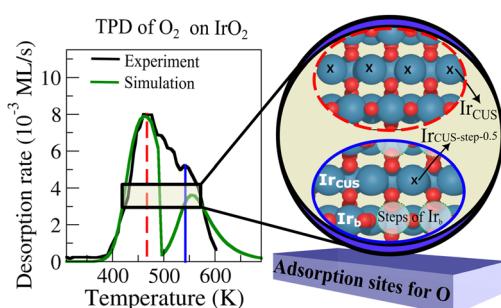
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**A combined AIMD and DFT study of the low-energy radiation responses of GaN**

Ming Jiang,\* Nuo Cheng, Xin-Yu Zhu, Xuan-Liang Hu, Zi-Han Wang, Ning Liu, Shuo Song, Sheng-Ze Wang, Xu-Sheng Liu\* and Chandra Veer Singh\*

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**Characterization of adsorption sites on  $\text{IrO}_2$  via temperature programmed  $\text{O}_2$  desorption simulations**

Vivianne K. Ocampo-Restrepo, Sudarshan Vijay, G. T. Kasun Kalhara Gunasooriya and Jens K. Nørskov\*

