

## IN THIS ISSUE

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### Cover

See Jesse Maassen, Erin R. Johnson *et al.*, pp. 16947–16954. Image reproduced by permission of Mohammad Rafiee Diznab from *Phys. Chem. Chem. Phys.*, 2024, 26, 16947.



### Inside cover

See Florentino López-Urías *et al.*, pp. 16955–16962. Image reproduced by permission of Florentino López-Urías from *Phys. Chem. Chem. Phys.*, 2024, 26, 16955.

## EDITORIAL

16929

### Physical chemistry of the energy transition

Robert Schlögl, Alec M. Wodtke, Timo Jacob and Svetlana Schauer mann



Timo Jacob (Ulm University)



Svetlana Schauer mann (Kiel University)

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



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



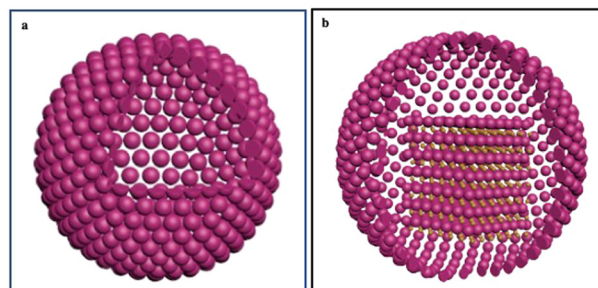
Alec Wodtke (Georg-August University & Department of Dynamics at Surfaces, Max-Planck-Institute for Multidisciplinary Sciences)

## PERSPECTIVE

16931

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

M. P. Pileni



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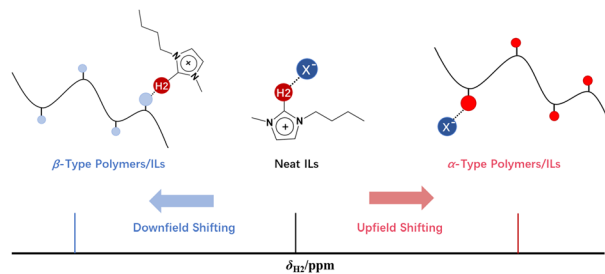


## COMMUNICATION

16942

### Polymer solubility mechanism in ionic liquids: $^1\text{H-NMR}$ spectra and two-parameter hydrogen bonding analysis

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

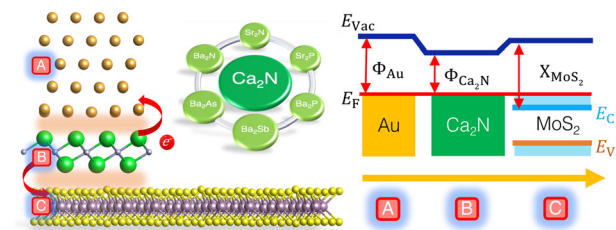


## RESEARCH PAPERS

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### Designing barrier-free metal/ $\text{MoS}_2$ contacts through electrone insertion

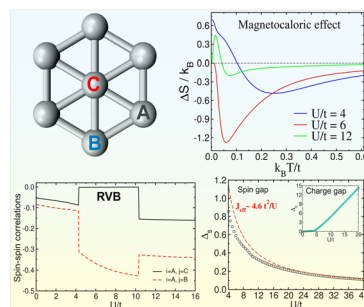
Mohammad Rafiee Diznab, Adrian F. Rumson, Jesse Maassen\* and Erin R. Johnson\*



16955

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

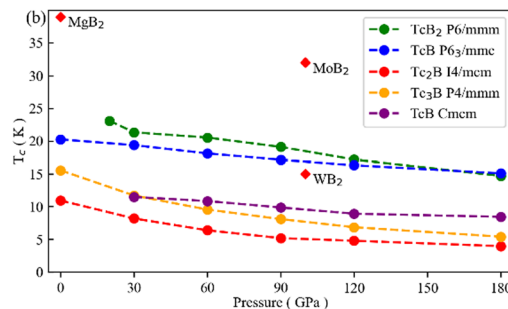
Florentino López-Urías,\* Alberto Rubio-Ponce, Emilio Muñoz-Sandoval and Francisco Sánchez-Ochoa



16963

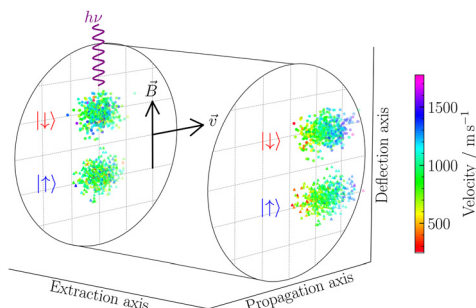
### Discovery of superconductivity in technetium borides at moderate pressures

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\*

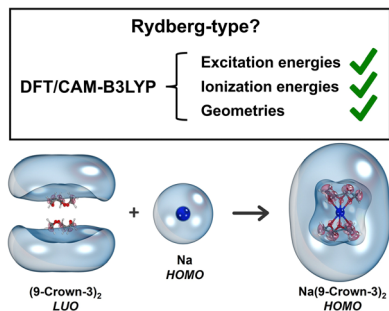
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### Tracking protein–protein interactions by NMR: conformational selection in human steroidogenic cytochrome P450 CYP17A1 induced by cytochrome $b_5$

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

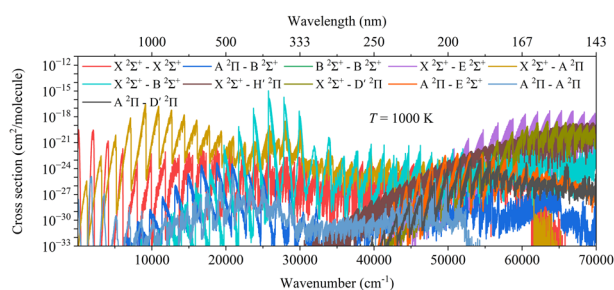
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### Electronic structure analysis and DFT benchmarking of Rydberg-type alkali-metal-crown ether, -cryptand, and -adamantane complexes

Isuru R. Ariyaratna

16998



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

Shuai Zhang, Zhi Qin and Linhua Liu\*

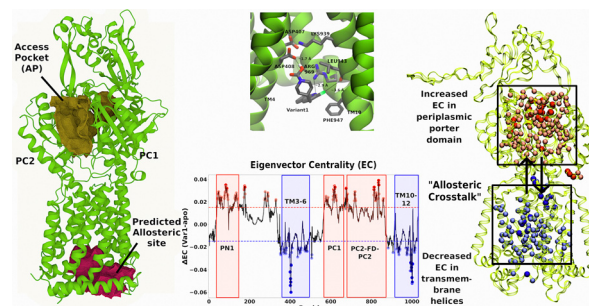


## RESEARCH PAPERS

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

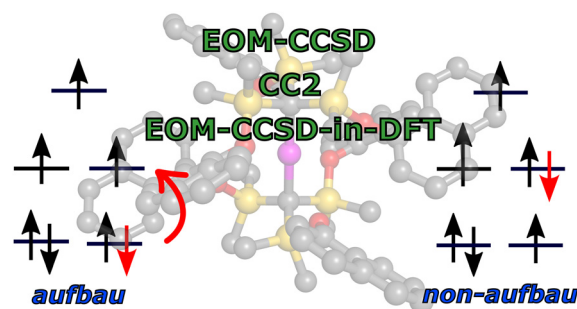
Abhishek Bera, Shreya Mukherjee and Niladri Patra\*



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

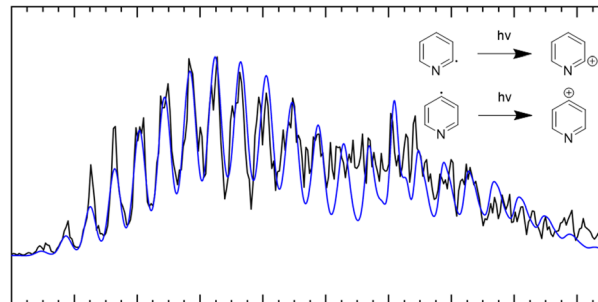
Maristella Alessio,\* Garrette Pauley Paran, Cansu Utku, Andreas Grüneis and Thomas-C. Jagau



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### Photoelectron spectrum of the pyridyl radical

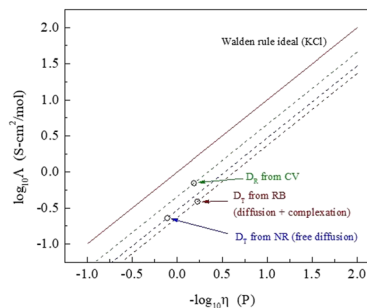
Emil Karaev, Marius Gerlach, Katharina Theil, Gustavo A. Garcia, Christian Alcaraz, Jean-Christophe Loison and Ingo Fischer\*



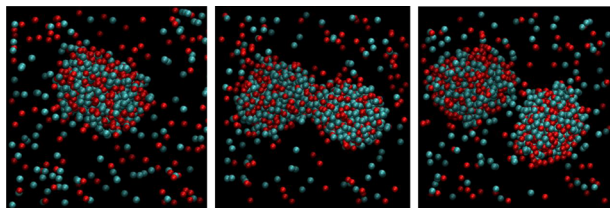
17048

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

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



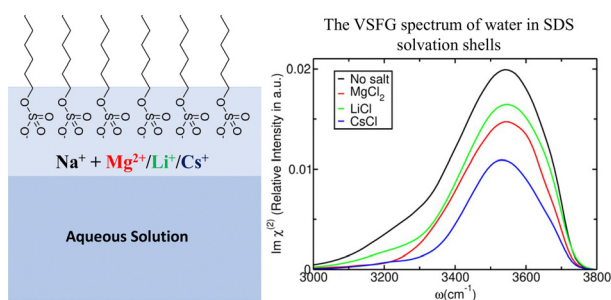
17057



### Secondary nucleation in symmetric binary SALR mixtures

Jiazheng Tan and Martin B. Sweatman\*

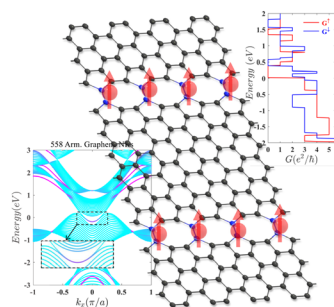
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### Effect of counterions on the structure and dynamics of water near a negatively charged surfactant: a theoretical vibrational sum frequency generation study

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

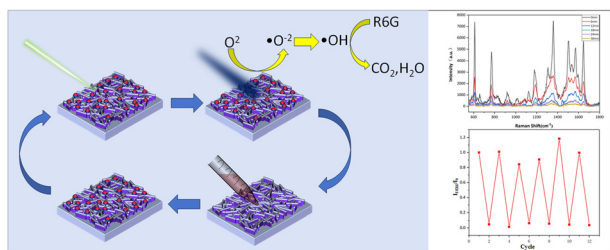
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### Topological phases, local magnetic moments, and spin polarization triggered by C<sub>558</sub>-line defects in armchair graphene nanoribbons

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

17083



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

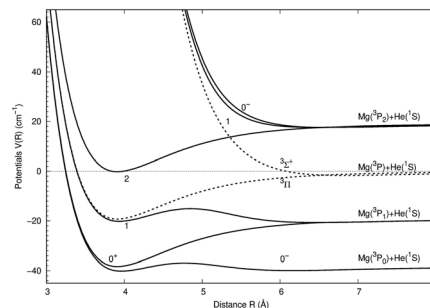
Jiale Zheng, Dongliang Liu, Xilong Liu, Zekai Wang, Junfeng Li, Xinxin Wang, Jun Wang, Qiang Fu, Yanqiang Cao, Liyong Jiang and Yikai Chen\*



17090

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

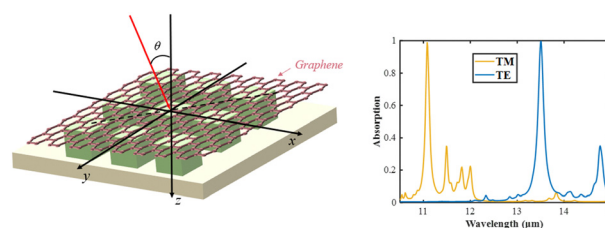
K. Alioua



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### A multi-dimensional photodetector based on an $\alpha\text{-MoO}_3$ grating and graphene

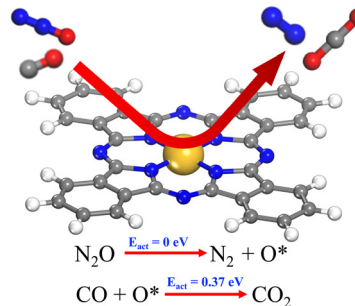
Yating Wang, Mingjun Wang,\* Haotuo Liu, Biyuan Wu, Xinyue Wang and Xiaohu Wu\*



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### Exploring Si-centered phthalocyanine as a single atom catalyst for $\text{N}_2\text{O}$ reduction: a DFT study

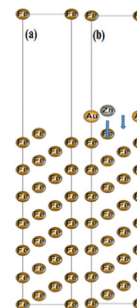
Adnan Ali Khan,\* Sarah Abdullah Alsalhi\* and Ata Ur Rahman



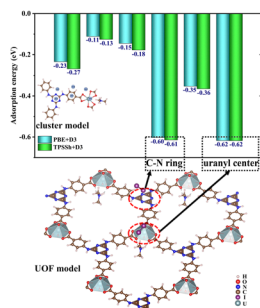
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### Adsorption and solar light activity of noble metal adatoms (Au and Zn) on Fe(111) surface: a first-principles study

Qaiser Rafiq, Muhammad Tahir Khan,\* Sardar Sikandar Hayat,\* Sikander Azam,\* Amin Ur Rahman, Hosam O. Elansary and Muhammad Shan



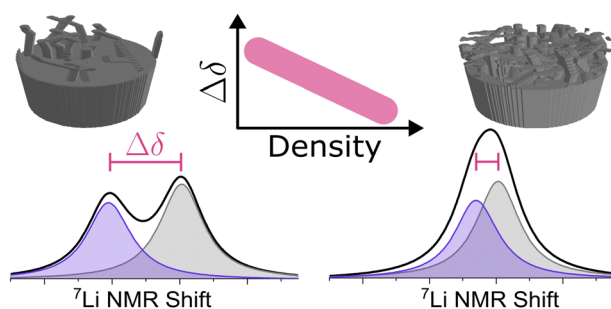
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### Iodine capture of a two-dimensional layered uranyl–organic framework: a combined DFT and AIMD study

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

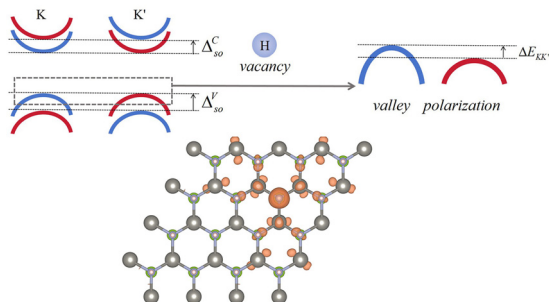
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### Morphology characterization of dendrites on lithium metal electrodes by NMR spectroscopy

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

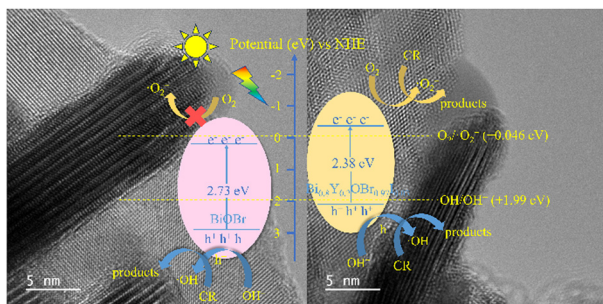
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### Large valley splitting and vacancy-induced valley polarization in two-dimensional WSeNH

Ziqi Wang, Xuening Han and Yan Liang\*

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### Enhancing the adsorption–photocatalytic efficiency of BiOBr for Congo red degradation by tuning the surface charge and bandgap via an Y<sup>3+</sup>–I<sup>–</sup> co-doping strategy

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



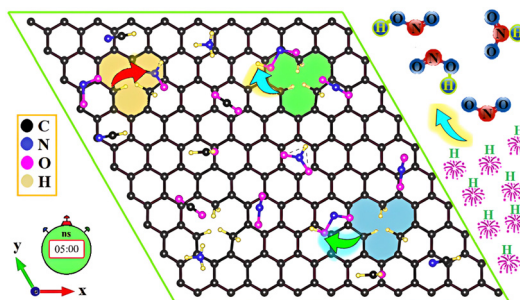


## RESEARCH PAPERS

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

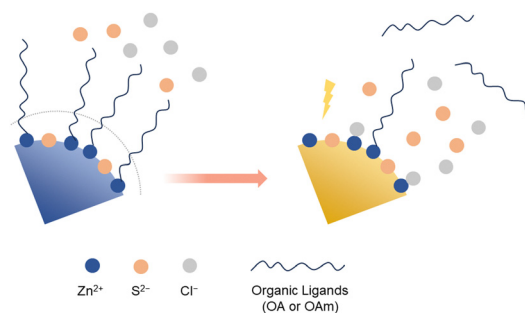
Nasim Hassani



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

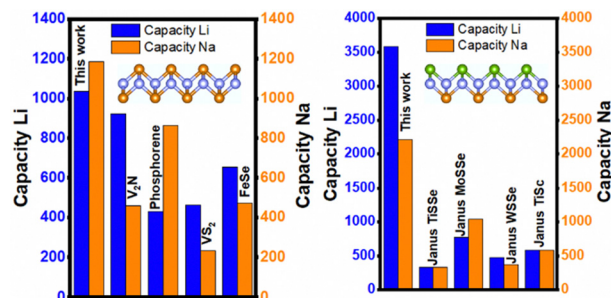
Zhe-Yong Chen, Xue Ren, Hui-Ling Hu, Meng Liu, Yi Liu and Feng-Lei Jiang\*



17191

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

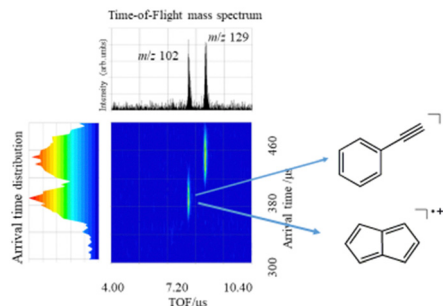
Dildar Ahmed, Nisar Muhammad and Z. J. Ding\*



17205

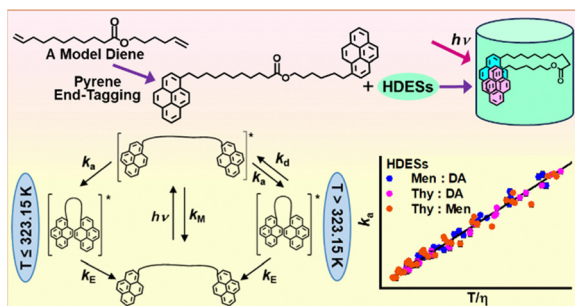
Structural analysis of C<sub>8</sub>H<sub>6</sub><sup>•+</sup> fragment ion from quinoline using ion-mobility spectrometry/mass spectrometry

Kenichi Iwamoto,\* Genki Inoue and Hiroshi Matsubara



## RESEARCH PAPERS

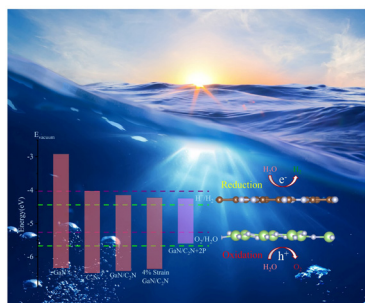
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## Assessing hydrophobic deep eutectic solvents for intramolecular excimer formation

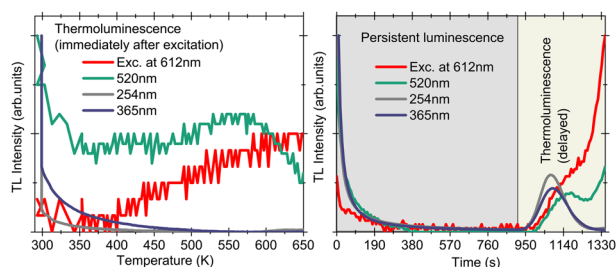
Shreya Juneja and Siddharth Pandey\*

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Doping and strain modulation of the electronic, optical and photocatalytic properties of the GaN/C<sub>2</sub>N heterostructure

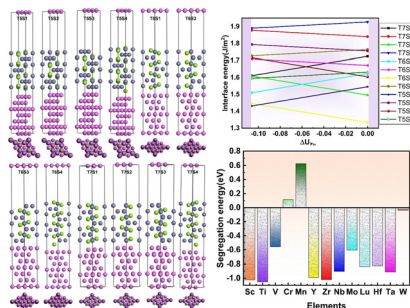
Fu Yin, Hui Wang,\* Zhengqin Zhao, LiJia Luo, Yongliang Tang, Yanbo Zhang and Qiang Xue

17232

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\*

17240

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

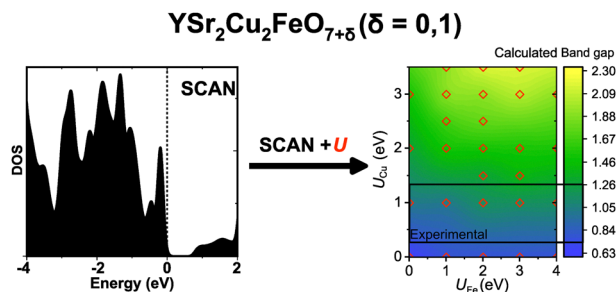
Qing Gao, Guoyu Qiao, Weibing Wang, Yuxiang Ge, Junqiang Ren, Wei Li, Ping Yang, Xuefeng Lu\* and Jisen Qiao\*



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

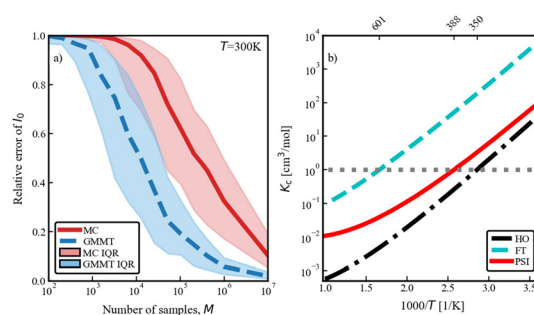
Marianela Gómez-Toledo and Elena M. Arroyo-de Dompablo\*



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

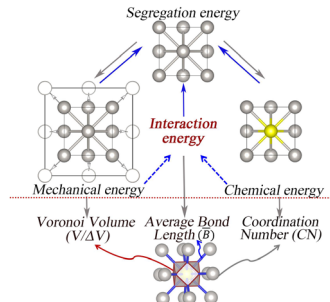
Katrin Blöndal, Kirk Badger, Khachik Sargsyan, David H. Bross, Branko Ruscic and C. Franklin Goldsmith\*



17274

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

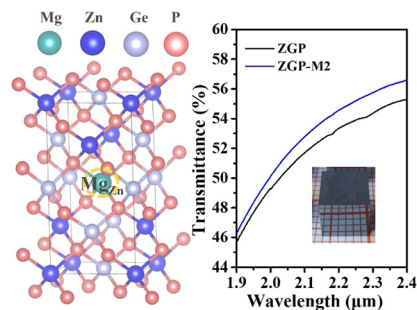
Xianxian Zhang, Jianfeng Tang,\* Xingming Zhang, Liang Wang, Dingwang Yuan, Huiqiu Deng and Lei Deng\*



17282

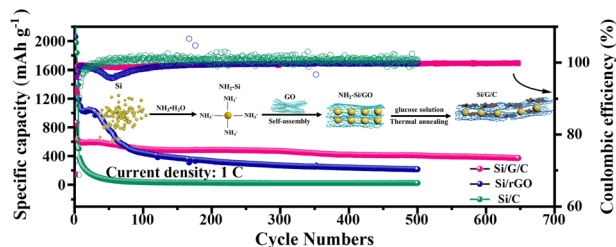
### Enhanced near-infrared optical transmission in zinc germanium phosphide crystals via precise magnesium doping

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



## RESEARCH PAPERS

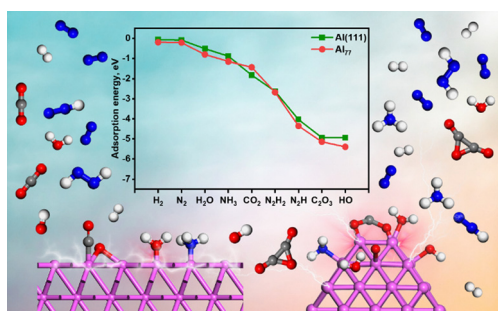
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### Carbon-coated silicon/graphite oxide composites as anode materials for highly stable lithium-ion batteries

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

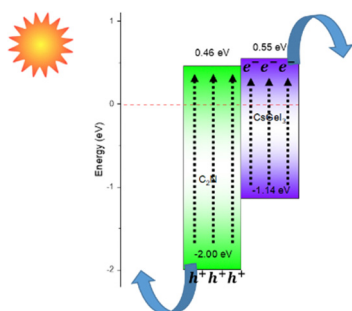
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### Adsorption mechanisms of decomposition species of CHON-containing explosives on aluminum surfaces

Kai Zhong and Chaoyang Zhang\*

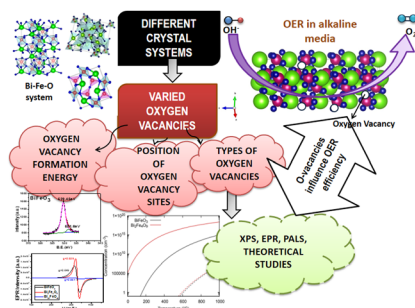
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### The lead-free perovskite-based heterojunction C<sub>2</sub>N/CsGeI<sub>3</sub>: an exploration for superior visible-light absorption

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

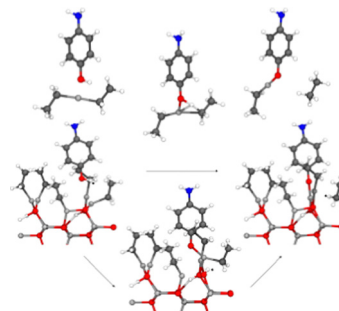
Shaswati Jyoti, Aditi Vijay, Umberto Terranova, Santosh K Gupta, Kathi Sudarshan and Sonalika Vaidya\*



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## Modelling the growth reaction pathways of zinc-oxide ALD/MLD hybrid thin films: a DFT study

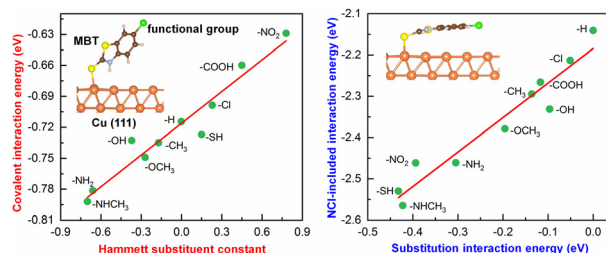
Mario Mäkinen,\* Timo Weckman and Kari Laasonen



17345

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

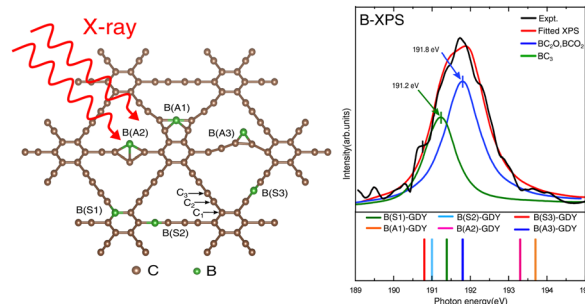
Thanh Hai Pham, Viorel Chihaiia and Do Ngoc Son\*



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

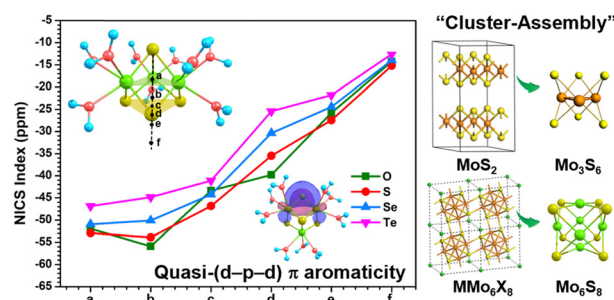
Hai-Bo Li, Jun-Rong Zhang,\* Xiu-Neng Song, Chuan-Kui Wang, Weijie Hua and Yong Ma\*



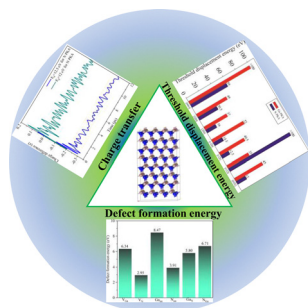
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## Revisiting the quasi-aromaticity in polynuclear metal chalcogenide clusters and their derivative "cluster-assembly" crystalline structures

Bochu Wang and Wan-Lu Li\*



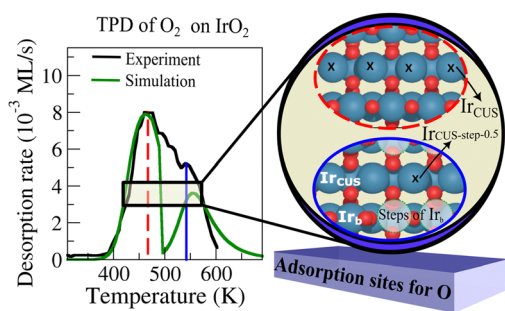
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### A combined AIMD and DFT study of the low-energy radiation responses of GaN

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 IrO<sub>2</sub> via temperature programmed O<sub>2</sub> desorption simulations

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

