

## IN THIS ISSUE

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**Cover**  
See Jesse Maassen, Erin R. Johnson *et al.*, pp. 6438–6446. Image reproduced by permission of Adrian F. Rumson from *Phys. Chem. Chem. Phys.*, 2025, 27, 6438.



**Inside cover**  
See Wenlong Xi and Patrick H.-L. Sit, pp. 6447–6456. Image reproduced by permission of Wenlong Xi and Patrick H.-L. Sit from *Phys. Chem. Chem. Phys.*, 2025, 27, 6447.

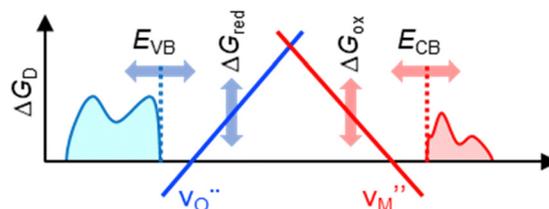
## TUTORIAL REVIEW

6390

### The physics of defect chemistry and the chemistry of defect physics

Andreas Klein\* and Denis Sudarikov

$$\Delta G_{\text{red}} = \Delta G_{v\ddot{O}} (\mu_{\text{O}} = 0, E_{\text{F}} = E_{\text{CB}}) + \frac{1}{2} \mu^{\text{O}}(\text{O}_2)$$

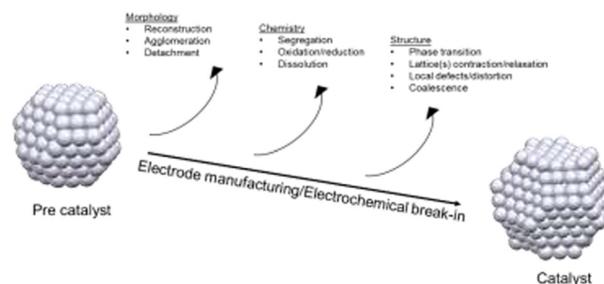


## PERSPECTIVES

6400

### Platinum-based nanoalloys for the oxygen reduction reaction: exposing the true active phase *via in situ/operando* techniques

Carlos A. Campos-Roldán,\* Raphaël Chattot, Pierre-Yves Blanchard, Deborah J. Jones and Sara Cavaliere\*



# RSC Applied Interfaces

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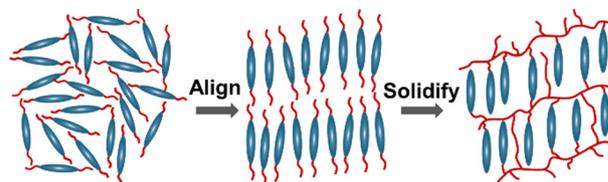
Fundamental questions  
Elemental answers

## PERSPECTIVES

6408

## Liquid crystals as solid-state templates

Nurjahan Khatun, Agnes C. Nkele and Kushal Bagchi\*

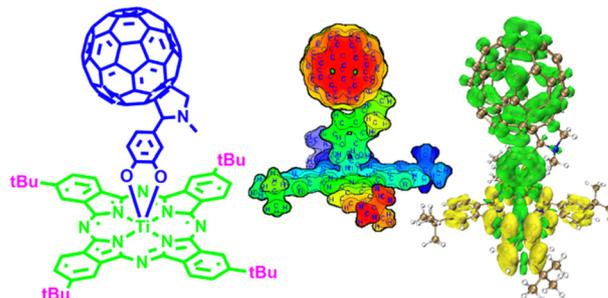


## COMMUNICATIONS

6425

The role of peripheral F-/H-atoms and *tert*-butyl substituents in charge transfer of axially substituted titanium phthalocyanines

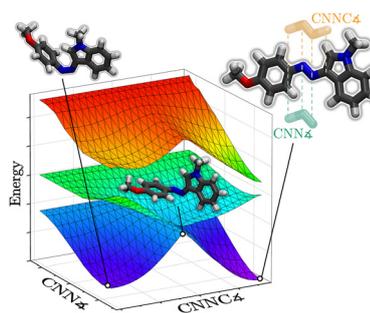
Ding Zhang, Yaochuan Wang,\* Haoran Ni, Xue Sun, Yizhuo Wang, Dajun Liu, Xuesong Xu and Yu Chen



6430

## Intramolecular subtleties in indole azo dyes revealed by multidimensional potential energy surfaces

Allen H. Chen, Zachary J. Knepp, Christian A. Guzman, Elizabeth R. Young\* and Lisa A. Fredin\*

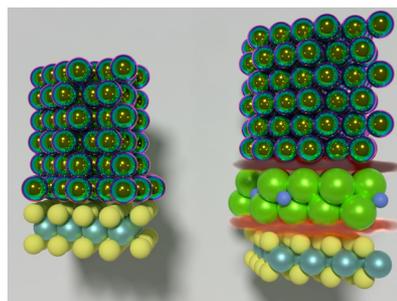


## RESEARCH PAPERS

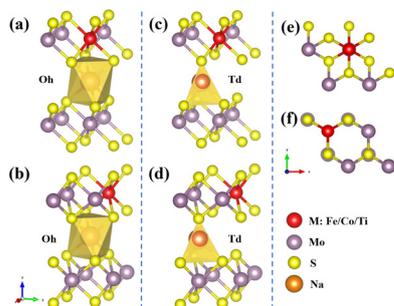
6438

The role of the metal in metal/MoS<sub>2</sub> and metal/Ca<sub>2</sub>N/MoS<sub>2</sub> interfaces

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



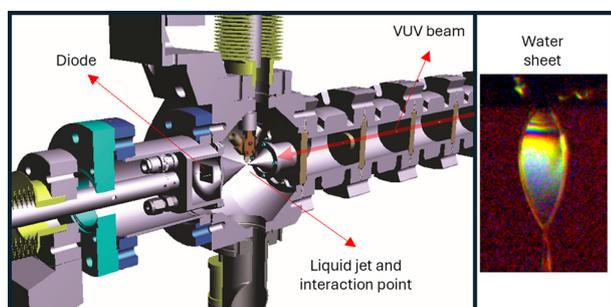
6447



### First-principles study of phase transition and the structural, energetic and electronic properties of pristine and transition metal (Fe/Co/Ti)-doped layered $\text{MoS}_2$ as anode materials for sodium-ion batteries

Wenlong Xi and Patrick H.-L. Sit\*

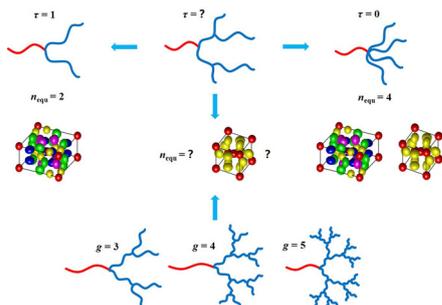
6457



### Ultrathin liquid sheets: water gets in shape for VUV absorption

Jonas Knurr, Patrick Hemberger, Patrick Ascher, Sven Augustin, David J. Hoffman, Gregor Knopp, Samuel Menzi, Zhibin Sun, Simon Tiefenbacher, Reto Wetter, Jake D. Koralek, Antoine Sarracini, Kirsten Schnorr, Christoph Bostedt, Andras Bodi\* and Andre Al Haddad\*

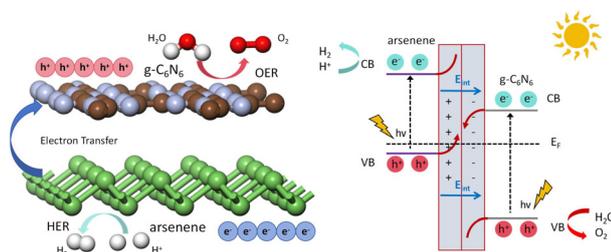
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### Effect of architectural asymmetry of hyperbranched block copolymers on their phase boundaries

Jiahao Shi, Qingshu Dong,\* Tao Yang and Weihua Li\*

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### Theoretical investigation of an arsenene/ $g\text{-C}_6\text{N}_6$ van der Waals heterojunction: a direct Z-scheme system with high photocatalytic efficiency

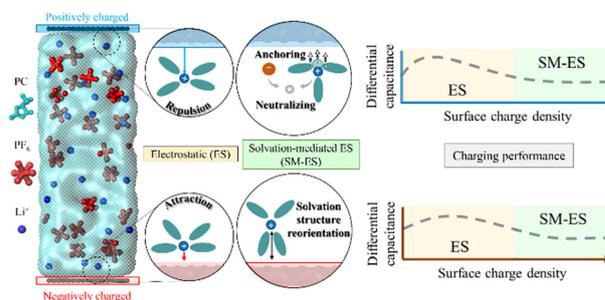
Zhengdong Sun, Jiaxin Ma, Junhao Zhu, Yifei Shen, Xiao Wang, Meng Zhang\* and Kaiyi Zhen\*



6486

### Solvation-mediated adsorption mechanism of solvated lithium ions at a charged solid–liquid interface for electrochemical energy storage: atomic scale investigation and insights

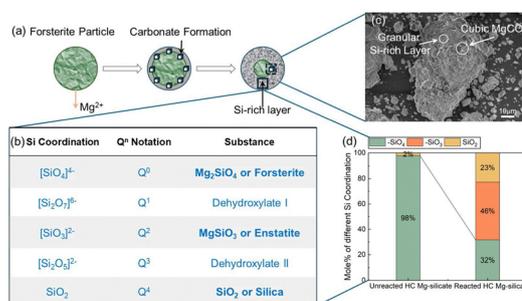
Muhammad Hamza, Bing-Ang Mei,\* Ridong Liao, Huihua Feng, Zhengxing Zuo, Zia ul Rehman Tahir and Rui Xiong



6500

### Evolution of silicate coordination in architected amorphous and crystalline magnesium silicates during carbon mineralization

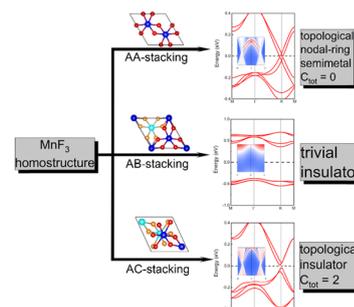
Xun Gao, Prince Ochonma, Divya Prasad, Mahadeo A. Mahadik, Ivan Kuzmenko, Jan Ilavsky and Greeshma Gadikota\*



6513

### Stacking induced symmetry breaking and gap opening in Dirac half-metal MnF<sub>3</sub>

Wentai Xiang and Baozeng Zhou\*



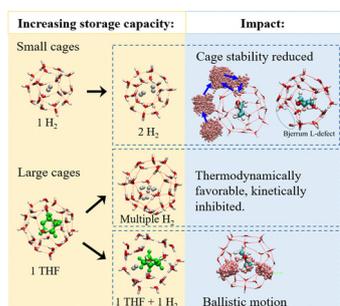
6523

### Gas-phase versus crystal structure of triflamide and some of its heterocyclic derivatives

Bagrat A. Shainyan,\* Alexey V. Eroshin and Sergey A. Shlykov\*



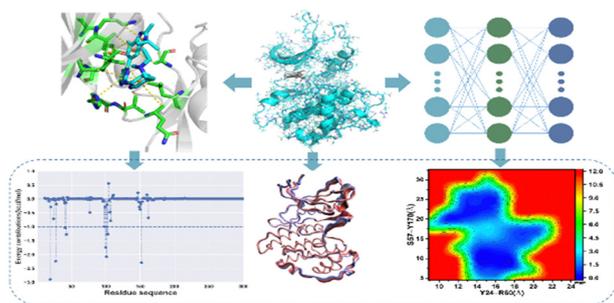
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### The effect of H<sub>2</sub> occupancy modes in small and large cages of H<sub>2</sub>-tetrahydrofuran hydrates on the hydrates' stability and H<sub>2</sub> storage capacity

Ruyi Zheng, Sohaib Mohammed, Yang Jia, Rituparna Hazra and Greeshma Gadikota\*

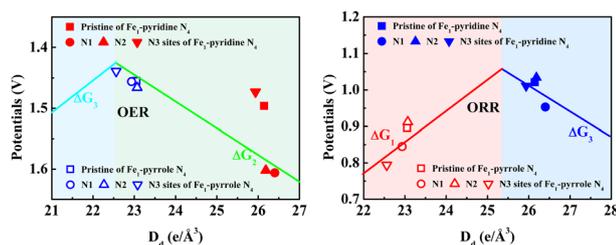
6546



### Insights into phosphorylation-induced influences on conformations and inhibitor binding of CDK6 through GaMD trajectory-based deep learning

Lu Zhao,\* Jian Wang, Wanchun Yang, Canqing Zhang, Weiwei Zhang and Jianzhong Chen\*

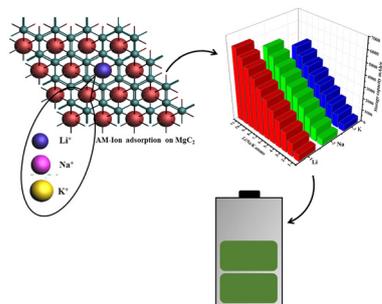
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### Tailoring OER/ORR activity in TM<sub>1</sub>N<sub>4</sub> catalysts through first-/second-shell nitrogen doping: a density functional theory investigation

Qingqing Cai, Wenmei Wuxia, HuanHuan Li, Can Li,\* Yinyan Gong, Lengyuan Niu and Tao Wang

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### A DFT study of monolayer magnesium carbide (MgC<sub>2</sub>) as a potential anode for (Li, Na, K) alkali metal-ion batteries

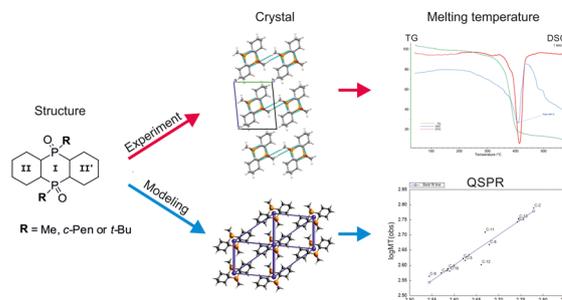
Muhammad Akbar, Noor ul Ain, Muhammad Isa Khan,\* Rajeh Alotaibi, Syed Mansoor Ali and Naveed Ashraf



6583

### Rationalization of the thermal properties of some polycyclic organophosphorus compounds by structural and QSPR analyses

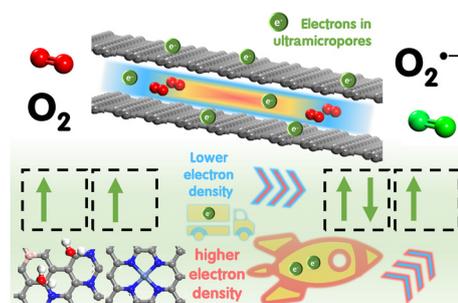
Elżbieta Łastawiecka, Marek Stankevič, Anna E. Kozioł, Joanna Matysiak, Konrad Dyk and Daniel M. Kamiński\*



6593

### Increasing the local electron density of carbons for enhanced O<sub>2</sub> activation at room temperature

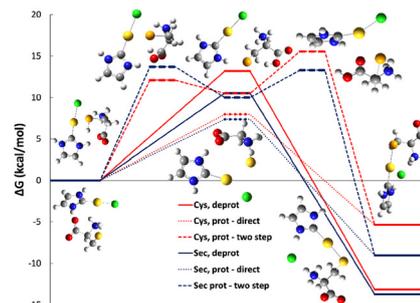
Yukun Pan, Hai Xu, Lekang Cui, Zhiqiang Zhao, Weibing Du, Jianghao Ye, Bo Niu, Yayun Zhang\* and Donghui Long



6604

### pH control of the reaction mechanism: interactions of the Au(I)-NHC complex with thioredoxin reductase (modeled by cysteine and selenocysteine); *ab initio* and DFT calculations

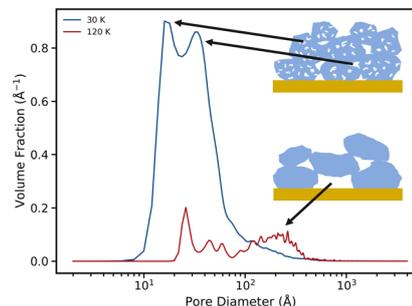
Filip Šebesta, Man Thi Hong Nguen, Markéta Munzarová and Jaroslav V. Burda\*



6616

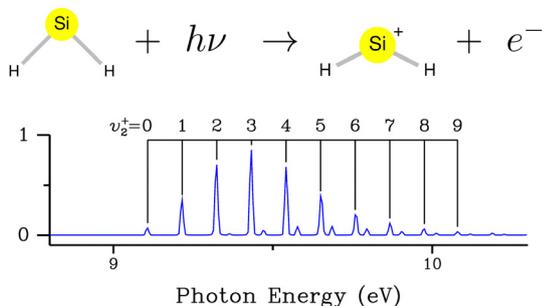
### Using neutrons to ascertain the impact of deposition temperature on amorphous solid water

Zachary Amato,\* Thomas F. Headen, Sabrina Gärtner, Pierre Ghesquière, Tristan G. A. Youngs, Daniel T. Bowron, Leide Cavalcanti, Sarah E. Rogers, Natalia Pascual, Olivier Auriacombe, Ellen Daly, Rachael E. Hamp, Catherine R. Hill, Ragesh Kumar TP and Helen J. Fraser



## RESEARCH PAPERS

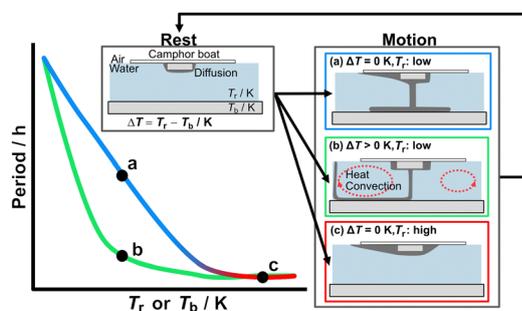
6628



### The threshold-photoelectron spectrum of SiH<sub>2</sub>: experiment and modeling with MCTDH method

L. H. Coudert,\* N. L. Chen, B. Gans, S. Boyé-Péronne, G. A. Garcia, S. Hartweg and J.-C. Loison

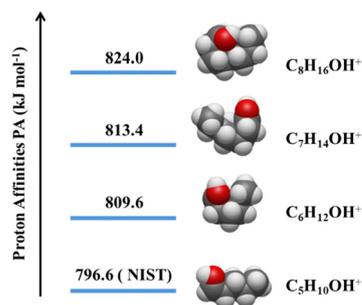
6640



### Oscillatory motion of a self-propelled object determined by the mass transport path

Masakazu Kuze, Nozomi Kawai, Muneyuki Matsuo,\* Istvan Lagzi, Nobuhiko J. Suematsu and Satoshi Nakata\*

6646



### Proton affinities of aldehyde molecules determined from the forward and backward gas-phase proton transfer reactions in a selected ion flow-drift tube

Maroua Omezzine Gnioua, Anatolii Spesyvyi and Patrik Španěl\*

6656



### An environmentally adaptive gold single-atom catalyst with variable valence states

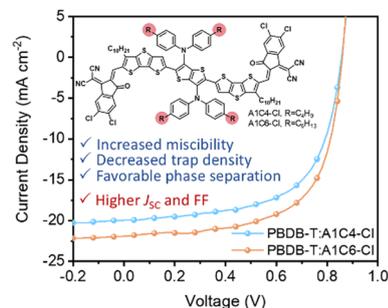
Meiliang Ma, Wen Liu, Xiaojuan Hu,\* Ying Jiang, Wentao Yuan, Zhong-Kang Han\* and Yong Wang



6663

### Optimizing the miscibility for enhanced photovoltaic performance of non-fused ring electron acceptors through side-chain engineering

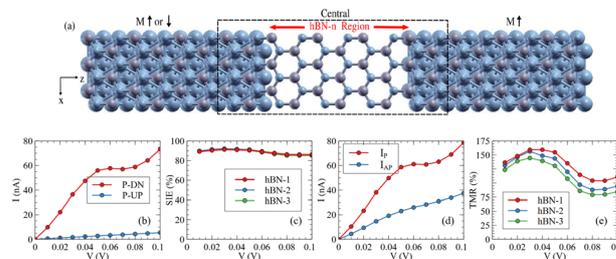
Yahui Bai, Linwei Xie, Zihui Lin, Qi Ai, Fuwen Zhao and Dan He\*



6669

### An *Ab initio* study on the enhancement of tunneling magnetoresistance and spin injection in Ni/vacuum/Ni magnetic tunnel junctions by h-BN stacking

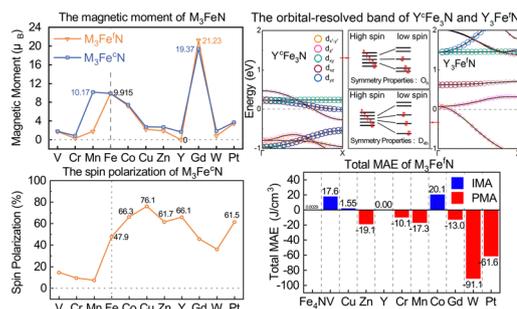
Ziqi Han, Chun-Sheng Liu, Xiaohong Zheng,\* Da-Yong Liu,\* Weiyang Wang\* and Yushen Liu



6677

### The emergence of novel magnetic properties in ternary iron nitrides toward spintronics: first-principles calculations

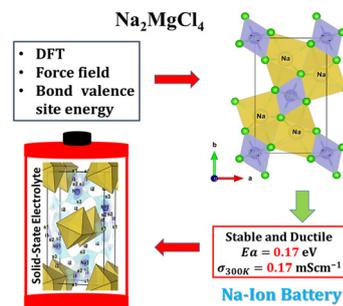
Ke Xiao, Xiaohui Shi,\* Xingyuan Zhang, Qingming Ping and Lulu Du\*



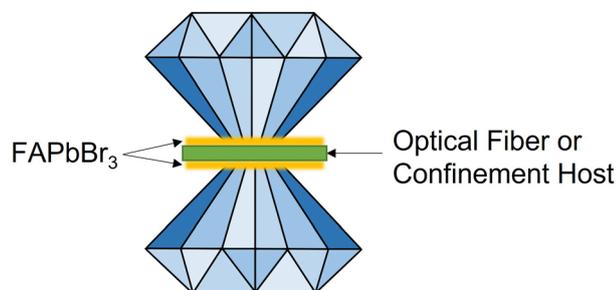
6687

### Theoretical evaluation of $\text{Na}_2\text{MgCl}_4$ double chlorite as an electrolyte for all-solid-state sodium-ion batteries

Yohandys A. Zulueta, Jose R. Fernández-Gamboa, Narciso Antonio Villar Goris, My Phuong Pham-Ho and Minh Tho Nguyen\*



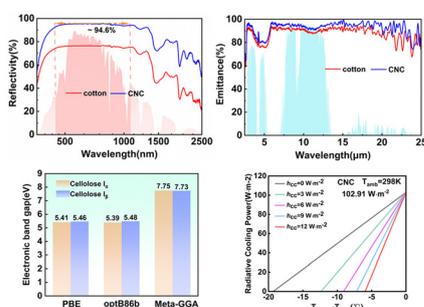
6698



### Enhanced structural stability of formamidinium lead bromide (FAPbBr<sub>3</sub>) perovskites in confined and coated configurations under varying pressures

Hai Yen Thi Nguyen, Duc Huy Nguyen, Chien-Chih Lai,\*  
Christopher M. Burba,\* Yuan-Cheng Chung and  
Hai-Chou Chang\*

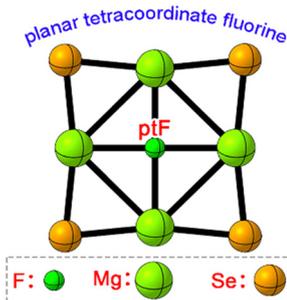
6710



### Physical insights into the high radiative cooling power of cellulose-based materials

Zhuo Zhao, Jian Zhang, Yuan Cheng, Aijun Hou,  
Yabei Xu, Daxin Liang\* and Gang Zhang\*

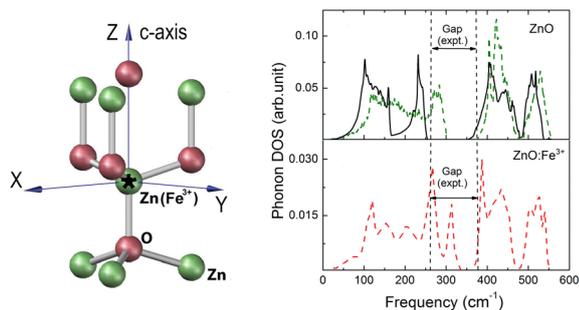
6718



### Planar tetracoordinate fluorine in a FMg<sub>4</sub>Se<sub>4</sub><sup>-</sup> cluster

Rui Sun, Caixia Yuan\* and Yan-Bo Wu\*

6724



### Optically active vibrations of extrinsic iron defects in zinc oxide

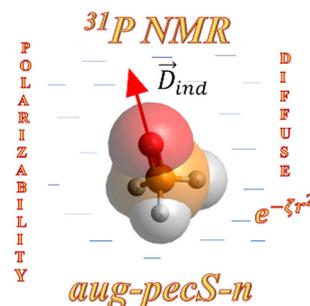
Alexey N. Kislov\* and Anatoly F. Zatsepin



6730

### Going beyond the routine consideration of solvent effects on $^{31}\text{P}$ NMR shielding constants: a meticulous basis set study and new aug-pecS- $n$ ( $n = 1$ and $2$ ) basis sets for phosphorus atoms

Yuriy Yu. Rusakov, Yuliya A. Nikurashina and Irina L. Rusakova\*



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### Macrocyclic meta-carborane hexamer. Evaluation of aromatic characteristics as a cluster-based analog to phenyl-bridged macrocyclic structures

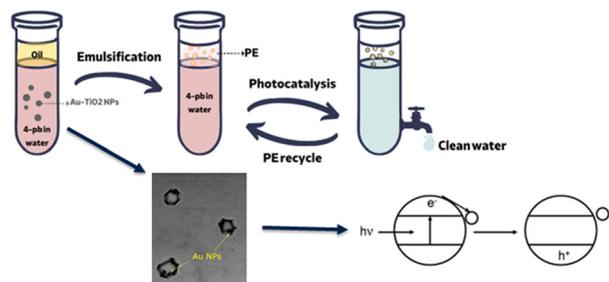
Peter L. Rodríguez-Kessler and Alvaro Muñoz-Castro\*



6751

### Dual-functional Au-TiO<sub>2</sub> nanoparticles: enhanced photocatalytic activity and Pickering emulsion stabilization for wastewater treatment

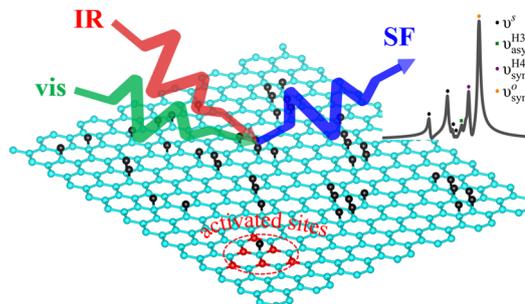
Zygimantas Gričius, Laurine Mroz and Gisle Øye\*



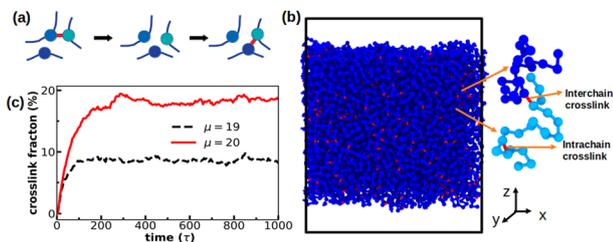
6766

### A theoretical study on the formation mechanism and the sum-frequency generation spectra of hydrogenated graphene

Shenghao Cui, Song Zhang, Qing Wang, Fumin Li, Zhitao Shen\* and Zhiying Ma\*



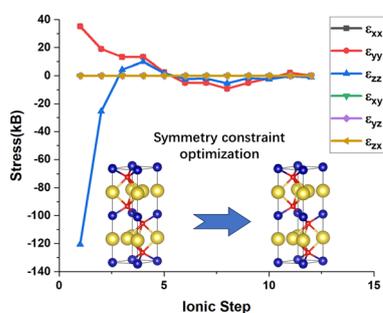
6777



### Rouse mode analysis of chain relaxation in reversibly crosslinked polymer melts

Rahul Karmakar, Srikanth Sastry, Sanat K. Kumar\* and Tarak K. Patra\*

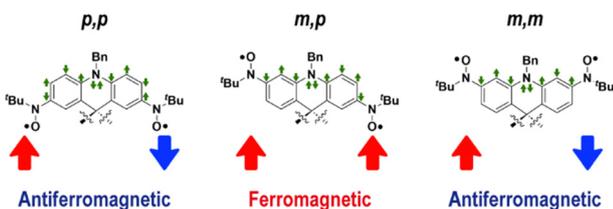
6786



### On-the-fly optimization of the lattice parameters with a symmetry constraint for high-throughput calculation

Shengyi Li, Li Xu,\* Cun Wang, Xuechun Wang, Yijie Hou, Peng Sheng, Huitao Bai, Hui Li, Qing Xue and Yumin Qian\*

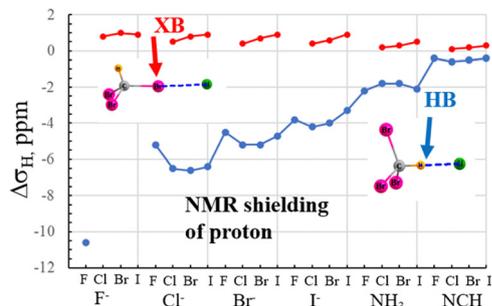
6794



### Radical site-dependent exchange interactions in acridane-based bisnitroxides

Yuta Takenouchi, Takuya Kanetomo\* and Masaya Enomoto\*

6800



### The competitive strengths of hydrogen and halogen bonding to haloforms and their different spectroscopic markers

Steve Scheiner



## CORRECTION

6810

**Correction: Achieving 9% EQE in light-emitting electrochemical cells *via* a TADF-sensitized fluorescence strategy**

Zeyang Zhou, Qingda Chang, Rui Chen, Pengfei Jin, Baipeng Yin,\* Chuang Zhang\* and Jiannian Yao

