

## IN THIS ISSUE

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**Cover**  
See Masaki Hanzawa, Ken-ichi Iimura *et al.*, pp. 6858–6866. Image reproduced by permission of Masaki Hanzawa from *Phys. Chem. Chem. Phys.*, 2025, 27, 6858.



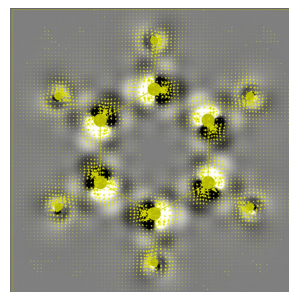
**Inside cover**  
See Michael R. Dooley and Shubham Vyas, pp. 6867–6874. Image reproduced by permission of Shubham Vyas from *Phys. Chem. Chem. Phys.*, 2025, 27, 6867.

## COMMUNICATIONS

6832

### Magnetically induced current density from numerical curls of nucleus independent chemical shifts

Raphael J. F. Berger\* and Maria Dimitrova\*

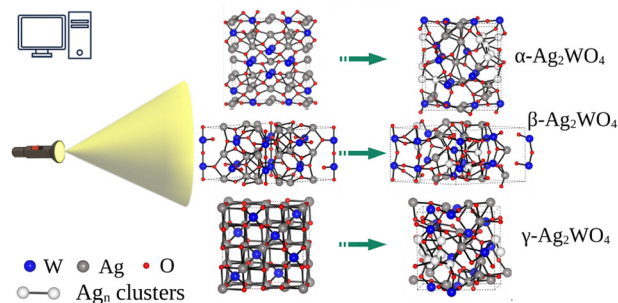


$$\vec{j} - \tilde{\vec{j}} = \frac{\nabla}{4\pi} \int \frac{\nabla' \cdot \tilde{\vec{j}}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}'$$

6836

### Lighting up the structure and electronic properties of $\alpha$ -, $\beta$ -, $\gamma$ - $\text{Ag}_2\text{WO}_4$ polymorphs under laser irradiation: a DFT investigation

L. Cabral,\* Elson Longo, Miguel A. San-Miguel, Edson Leite, E. Z. da Silva and Juan Andrés\*



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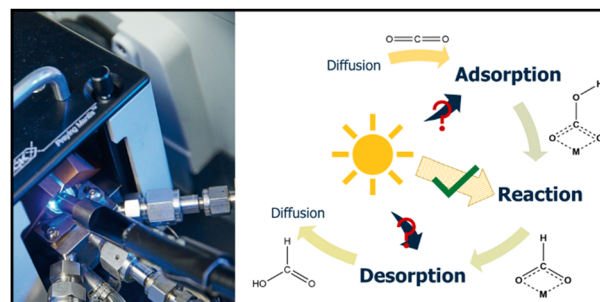
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## COMMUNICATIONS

6845

### Influence of light on ad- and desorption processes on titanium dioxide surfaces towards efficient CO<sub>2</sub> photoreduction

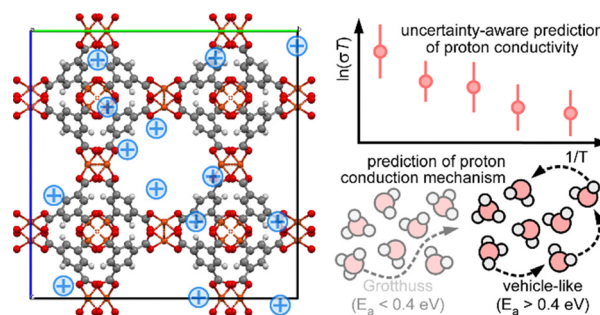
Pawel Naliwajko, Nikolaos G. Moustakas, Marcus Klahn, Tim Peppel and Jennifer Strunk\*



6850

### Examining proton conductivity of metal–organic frameworks by means of machine learning

Ivan V. Dudakov, Sergei A. Savelev, Iurii M. Nevolin, Artem A. Mitrofanov, Vadim V. Korolev\* and Yulia G. Gorbunova

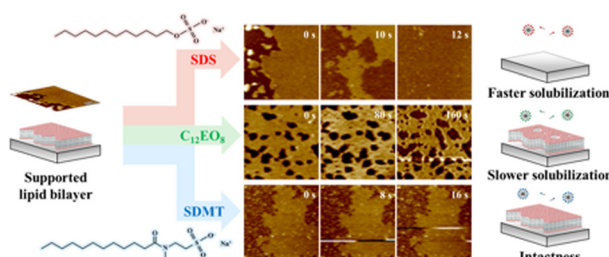


## RESEARCH PAPERS

6858

### Direct observation of interactions between supported lipid bilayers and surfactants

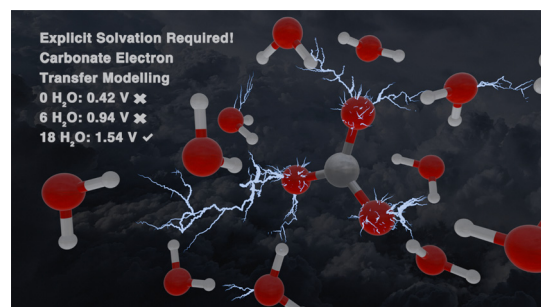
Masaki Hanzawa,\* Hiroaki Sugawara, Taku Ogura, Ken-ichi Iimura\* and Takeshi Misono



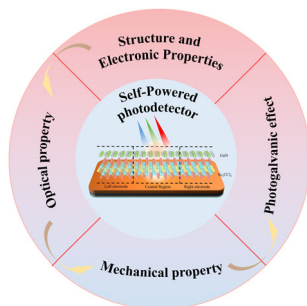
6867

### Role of explicit solvation and level of theory in predicting the aqueous reduction potential of carbonate radical anion by DFT

Michael R. Dooley and Shubham Vyas\*



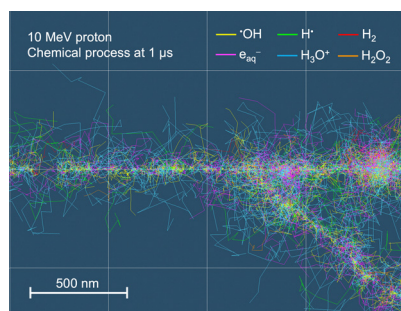
6875



### Self-powered photodetector of GaN/Sc<sub>2</sub>CCl<sub>2</sub> heterojunction with high carrier mobility and polarization sensitivity

Guoqing Zhang, Zhen Cui,\* Aming Song, Shuang Zhang and Lu Wang

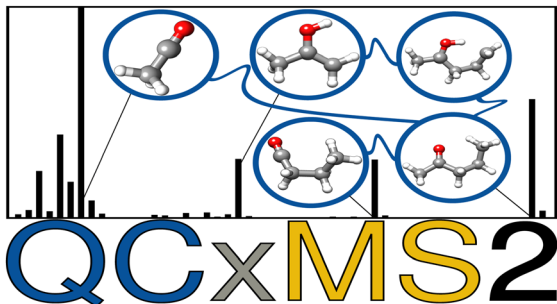
6887



### Development of a chemical code applicable to ions based on the PHITS code for efficient and visual radiolysis simulations

Yusuke Matsuya,\* Yuji Yoshii, Tamon Kusumoto, Tatsuhiko Ogawa, Seiki Ohnishi, Yuho Hirata, Tatsuhiko Sato and Takeshi Kai

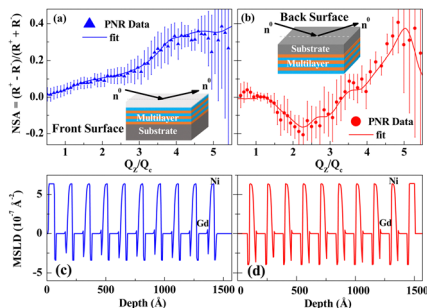
6899



### QCxMS2 – a program for the calculation of electron ionization mass spectra *via* automated reaction network discovery

Johannes Gorges and Stefan Grimme\*

6912



### Experimental realization of a helical magnetic structure at Ni/Gd interfaces at room temperature

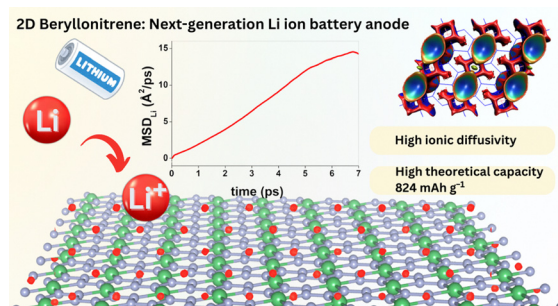
Surendra Singh,\* Harsh Bhatt, D. Sarkar and M. Gupta



6924

### Exploring the potential of 2D beryllonitrene as a lithium-ion battery anode: a theoretical study

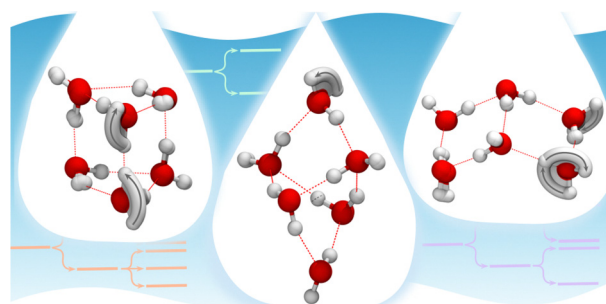
Antara Vaidyanathan, Harkishan Dua, Utpal Sarkar, Nicola Seriani\* and Brahmananda Chakraborty\*



6938

### Tunneling splittings in the energetically low-lying structural isomers of the water hexamer: the prism, the cage and the book

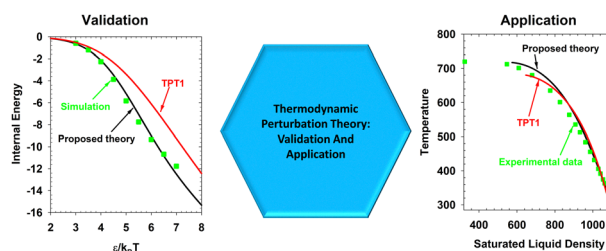
Nina Tokić, Mihael Eraković and Marko T. Cvitaš\*



6958

### Advanced association theory for monoethylene glycol: thermodynamic perturbation theory, Monte Carlo simulation, and equation of state parametrization

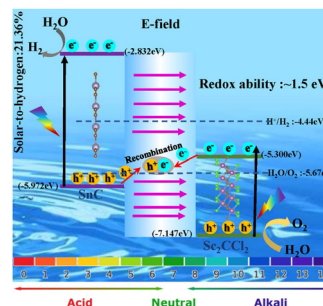
Mahmood Abdi and Hassan Hassanzadeh\*



6976

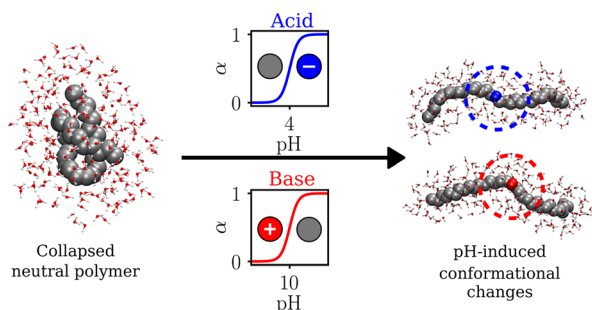
### Z-Scheme heterostructures of 2D SnC/Sc<sub>2</sub>CCl<sub>2</sub> for overall water splitting with strong redox potential under visible light

Xingyong Huang,\* Mingjie Wan, Qilong Cao, Hai-Zhi Song and Ming Yang



## RESEARCH PAPERS

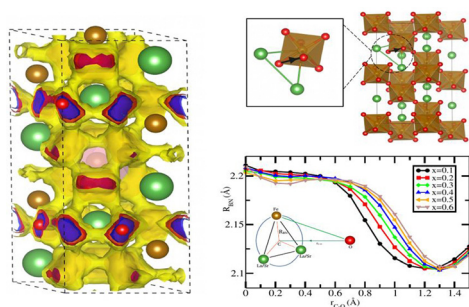
6984



### A generic model for pH-sensitive collapse of hydrophobic polymers

Varun Mandalaparthi\* and Nico F. A. van der Vegt

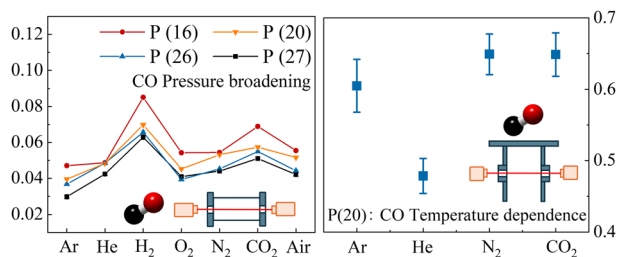
6994



### Molecular dynamics studies of oxide ion transport in Sr-doped LaFeO<sub>3</sub>: role of cationic environments and cooperativity

Sanjib Ray and P. Padma Kumar

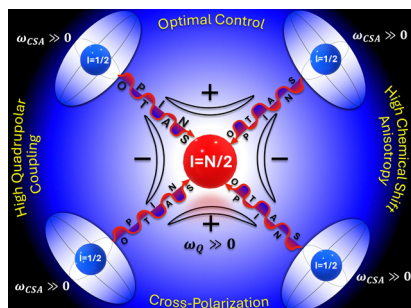
7004



### Measurement of carbon monoxide pressure broadening and temperature dependence coefficients in the 1 ← 0 band

Denghao Zhu,\* Leopold Seifert, Sumit Agarwal, Bo Shu, Ravi Fernandes and Zhechao Qu\*

7016



### Optimal control-based nuclear spin cross-polarization in the presence of complicating anisotropic interactions

Shovik Ray, Venkata SubbaRao Redrouthu, Asif Eqbal and Sheetal Kumar Jain\*

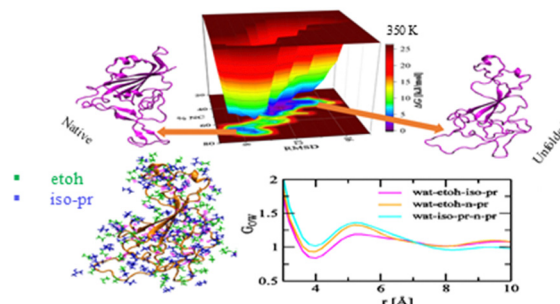


## RESEARCH PAPERS

7028

## Unraveling the impact of binary vs. ternary alcohol solutions on the conformation and solvation of the SARS-CoV-2 receptor-binding domain

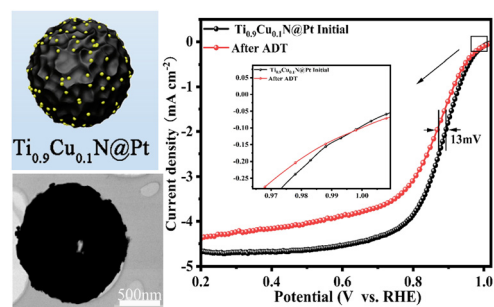
Rabiul Gazi and Madhurima Jana\*



7044

Designed synthesis of multi-defective  $\text{Ti}_{0.9}\text{Cu}_{0.1}\text{N@Pt}$  as a robust catalyst for the oxygen reduction reaction

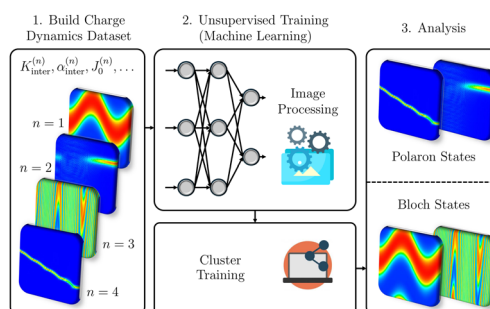
Sipeng Chen, Jiquan Lu, Yuying Li, Yuying Zheng\* and Ting Zhu\*



7053

## Determining charge transport regimes in organic molecular crystals: a machine learning framework

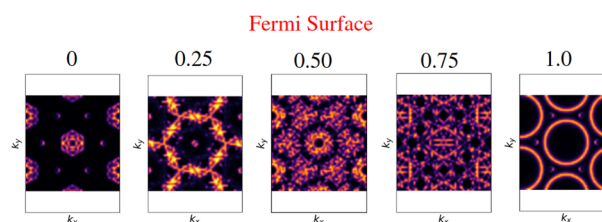
T. S. A. Cassiano, M. L. Pereira Junior, P. H. de Oliveira Neto\* and L. A. Ribeiro Junior



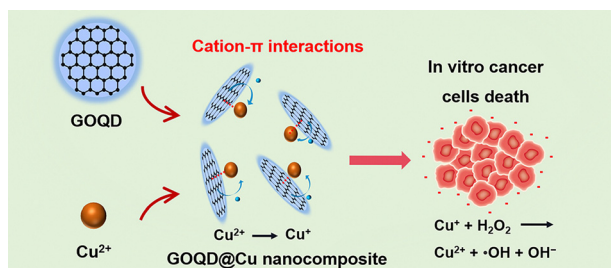
7068

## The influence of interlayer bias and crystal field on the electronic characteristics of twisted tri-layer graphene

Mufasila Mumthaz Muhammed and Junais Habeeb Mokkaath\*



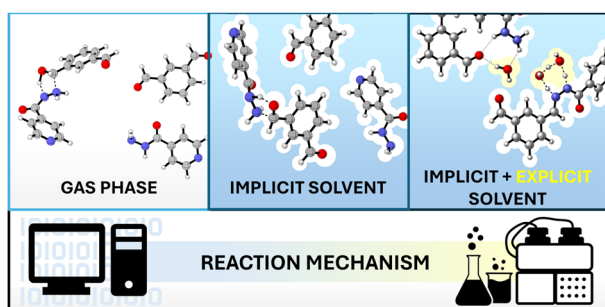
7076



### Enhanced anticancer activity of graphene oxide quantum dot@Cu nanocomposites via cation- $\pi$ interactions

Fangxiao Li, Ran Guo, Yinwei Qiu, Zhengyang Liu, Lingling Tao, Shouning Yang, Junjie Chen\* and Huayan Yang\*

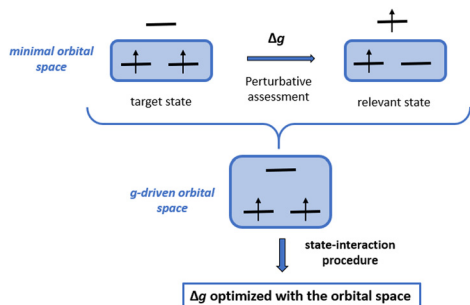
7084



### Mechanistic insights on hydrazones synthesis: a combined theoretical and experimental study

Nissrine Al Assaad, Alain Chamayou, Rachel Calvet,\* Manuel Pedrón,\* Ilaria Ciofini and Frédéric Labat\*

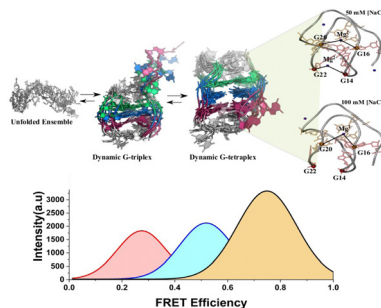
7093



### Efficient state-interaction approach for the g-matrix analysis in high-spin molecules

Antonio Cebreiro-Gallardo and David Casanova\*

7104



### Emergence of a dynamic G-tetraplex scaffold: uncovering low salt-induced conformational heterogeneity and the folding mechanism of telomeric DNA

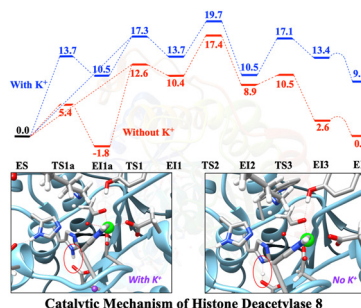
Manali Basu, Avijit Mainan, Susmita Roy\* and Padmaja Prasad Mishra\*



7120

### Deacetylation mechanism of histone deacetylase 8: insights from QM/MM MP2 calculations

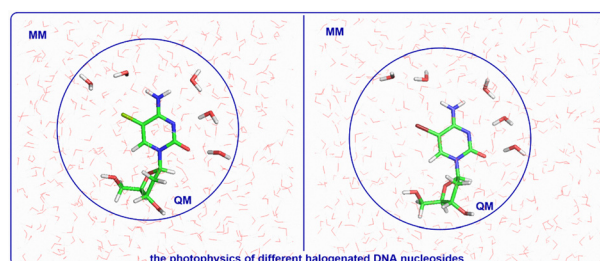
Rui Lai\* and Hui Li\*



7139

### Quantum mechanics/molecular mechanics studies on mechanistic photophysics of epigenetic C5-halogenated DNA nucleosides: 2'-deoxy-5-chlorocytidine and 2'-deoxy-5-bromocytidine in aqueous solution

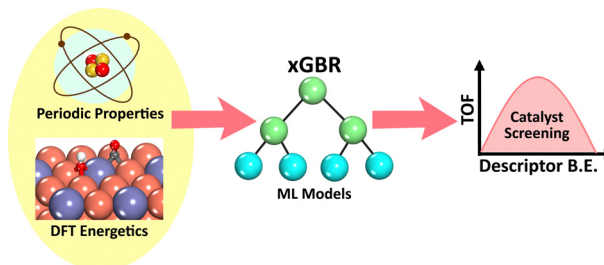
Xue-Ping Chang,\* Feng-Ran Fan, Ke Liu, Hai-Ting Lv, Geng Zhao, Lingyun Zheng, Teng-Shuo Zhang and Bin-Bin Xie



7151

### Machine learning assisted approximation of descriptors (CO and OH) binding energy on Cu-based bimetallic alloys

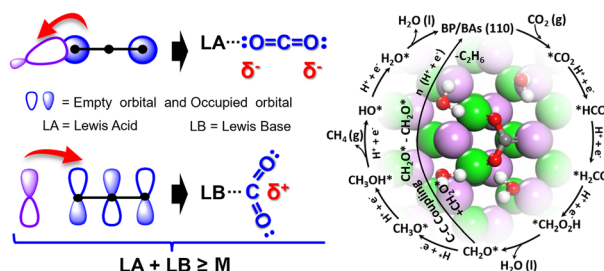
Pallavi Dandekar, Aditya Singh Ambesh, Tuhin Suvra Khan and Shelaka Gupta\*



7169

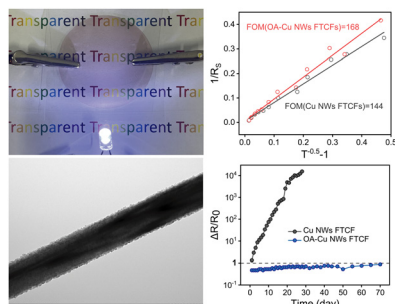
### Tailoring frustrated Lewis pair catalysts for enhanced electrochemical CO<sub>2</sub> reduction to multi-carbon fuels

Li Shi, Zhengyu Gu, Peng Wu, Xiaobing Wang, Jingzhuo Zhou, Xiuyun Zhang,\* Yanwen Ma\* and Jin Zhao\*



## RESEARCH PAPERS

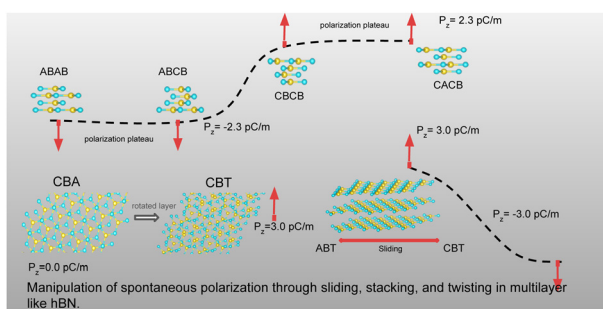
7177



### High initial conductivity and oxidation resistance of copper nanowire films via depositing oxalic acid

Weiqliang Yuan, Xingzhong Zhu,\* Jizhe Zhang, Juan Xu, Yuhao Zhang, Junyao Cai, Ning Peng and Caixia Kan\*

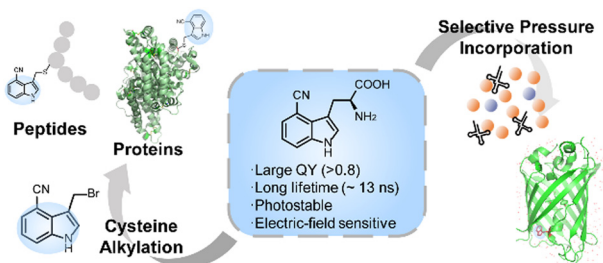
7189



### Slide and twist: manipulating polarization in multilayer hexagonal boron-nitride

Sanber Vizcaya,\* Felipe Pérez Riffo, Juan M. Florez and Eric Suárez Morell

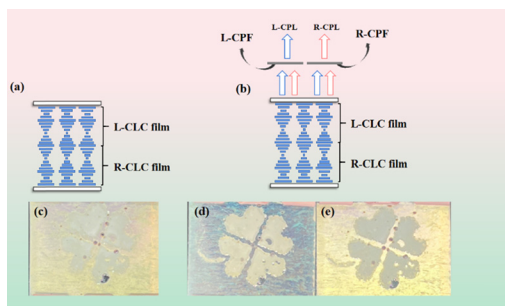
7199



### Chemical and biological incorporation of the blue fluorescent amino acid 4-cyanotryptophan into proteins: application to tune the absorption and emission wavelengths of GFP

Manxi Wang and Feng Gai\*

7205



### Cholesteric liquid crystal based polymer anti-counterfeit lamination films with broadband hyper-reflective properties and effective shielding against infrared laser beams

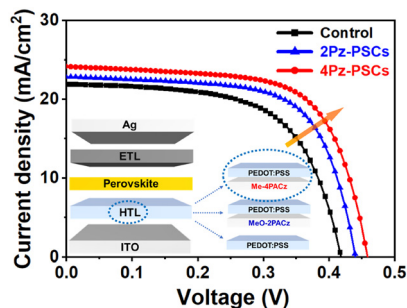
Yutong Liu, Mengqi Xie, Yue Cao, Zhidong Liu, Zhou Yang, Dong Wang, Wanli He, Hui Cao,\* Huihui Wang\* and Guang Cui\*



7215

### Interface modification of hole transport layers in tin-based halide perovskite solar cells

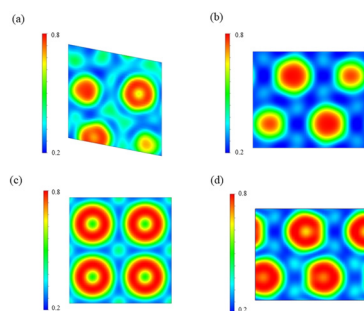
Xin Zhang, Xinyao Chen, Zhenjun Li, Jin Cheng, Chunqian Zhang and Junming Li\*



7225

### Predictions of an ambient stable uranium and a superhard uranium

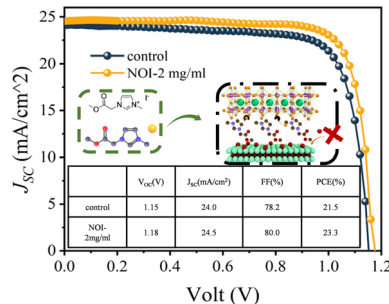
Xiaoshang Wen, Runqing Zhang, Junzhao Li, Jingyi Zhang, Haijie Zhang, Huafeng Dong,\* Renhai Wang, Yujue Yang and Fugen Wu



7232

### Multifunctional small molecule interface management for efficient planar perovskite solar cells

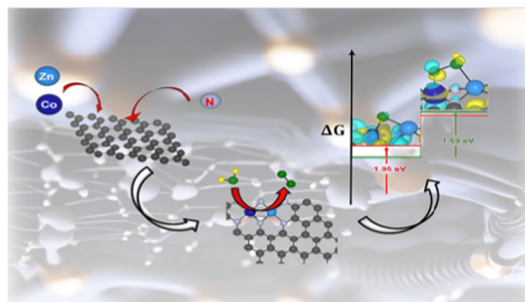
Rui Zhou, Xin Hu, Haijin Li, Huiyao Zhao, Yanbei Wei, Jun Qu, Yangdi Chen, Liping Su, Longhao Jisi and Wenfeng Zhang\*



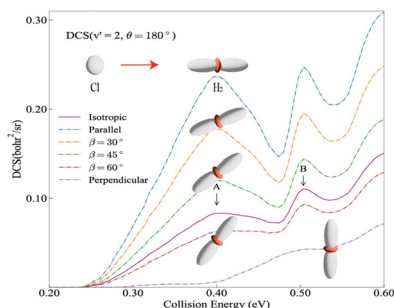
7240

### Deciphering the impact of Zn-incorporation on M-NC (M = Fe, Co, Ni, Cu) type catalysts for enhanced HER and OER performance

Saptarshi Ghosh Dastider, Krishna Kanta Haldar and Krishnakanta Mondal\*



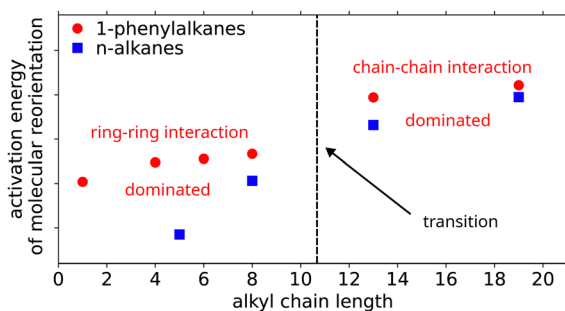
7250



### Stereodynamical control of resonances in the $\text{Cl} + \text{H}_2 (\nu = 1, j = 1) \rightarrow \text{HCl} + \text{H}$ reaction

Xiaoxi Xu, Bayaer Buren\* and Maodu Chen\*

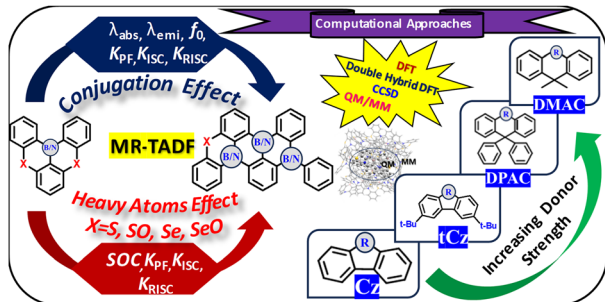
7258



### On the relation of structure and dynamics in aromatic ring-tail structured liquids

Rolf Zeißler,\* Jan Philipp Gabriel, Dorte Posselt and Thomas Blochowicz

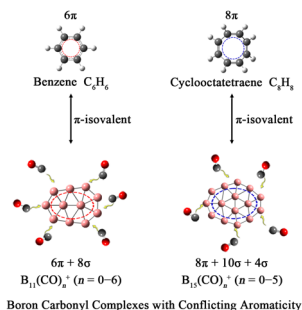
7265



### A theoretical investigation of heavy atom and oxidation effects in MR-TADF emitters for OLEDs: a combined DFT, double hybrid DFT, CCSD, and QM/MM approaches

Singaravel Nathiya, Murugesan Panneerselvam\* and Luciano T. Costa\*

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### Observation of boron carbonyl complexes $\text{B}_{11}(\text{CO})_n^+$ ( $n = 1-6$ ) and $\text{B}_{15}(\text{CO})_n^+$ ( $n = 1-5$ ) with conflicting aromaticity

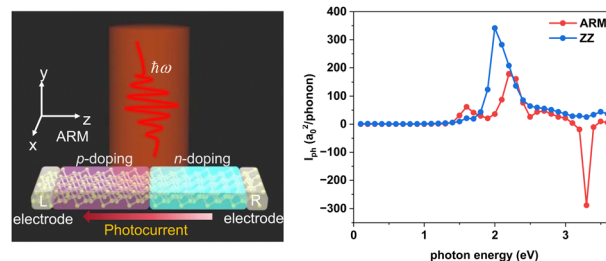
Rui-Nan Yuan, Qiang Chen,\* Hong Niu, Cai-Yue Gao, Xiao-Ni Zhao, Yan-Bo Wu, Sheng-Gui He\* and Si-Dian Li\*



7288

### First-principles analysis of the photocurrent in a monolayer $\alpha$ -selenium p–n junction optoelectronic device

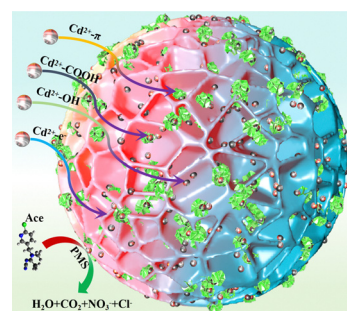
Yuqian Wang, Xiaoyong Xiong, Shibo Fang, Hong Li, Zhulin Weng, Dahua Ren and Qiang Li\*



7296

### Mechanism study on the removal of $\text{Cd}^{2+}$ and acetamidrid from wastewater treatment plant effluent by PMS activated by tobacco stem biochar under humic acid induction

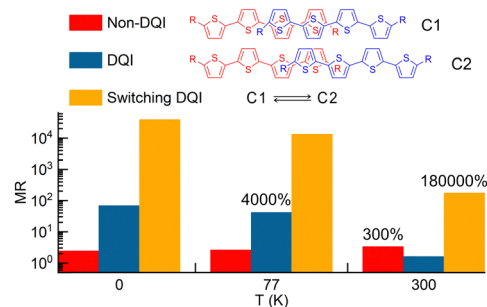
Xiaojuan Su, Pengfei Gao, Yuanchuan Ren,\* Jieba Li and Nanqi Ren\*



7309

### Molecular magnetoresistance enhanced by destructive quantum interference of a $[\pi \cdot \cdot \pi]$ supramolecule

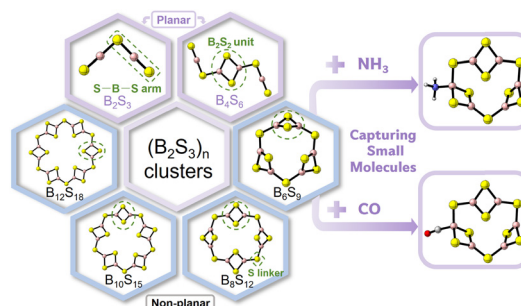
Hua Hao,\* Shuhui Qin, Ting Jia\* and Xiaohong Zheng



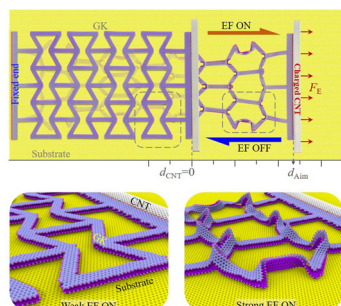
7317

### Structural evolution and electronic properties of boron sulfides $(\text{B}_2\text{S}_3)_n$ ( $n = 1-6$ ): insights from DFT calculations

Jingxin Hu, Lin Zhang and Zexing Cao\*



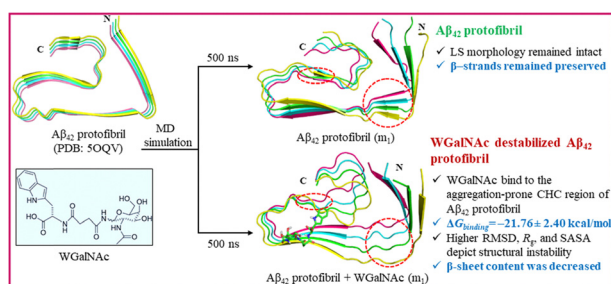
7326



## A high-frequency nanoscale positioner driven by an external electric field: a molecular dynamics study

Huichang Feng, Kun Cai,\* Jiao Shi and Yingyan Zhang\*

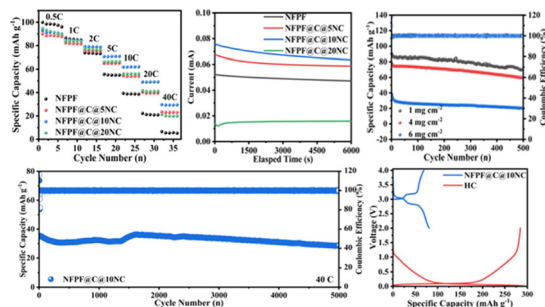
7336



## Delineating the tryptophan–galactosylamine conjugate mediated structural distortions in Aβ<sub>42</sub> protofibrils

Arushi Dabas and Bhupesh Goyal\*

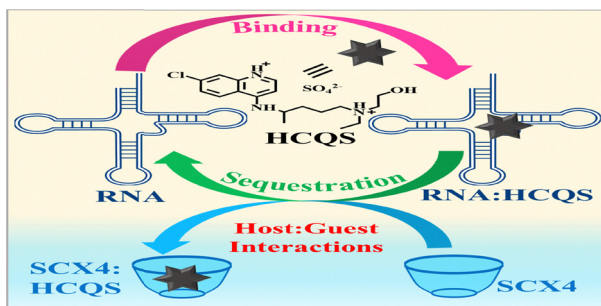
7356



## Enhanced electrochemical performance of N-doped carbon coated Na<sub>2</sub>FePO<sub>4</sub>F cathode materials for sodium-ion batteries: achieving high capacity and cycle stability

He Zhang, Mian Zhao, Zhixuan Yu, Tengwei Ma, Hailong Qiu\* and Di Jin\*

7365



## Probing the nucleobase-specific binding interaction of hydroxychloroquine sulfate with RNA and subsequent sequestration by a water-soluble molecular basket

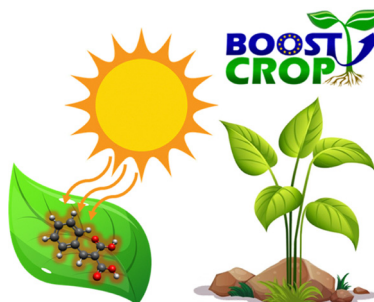
Rahul Yadav, Subhasis Das, Madhumita Mukherjee and Saptarshi Mukherjee\*



7375

### Molecular heaters: a green route to boosting crop yields?

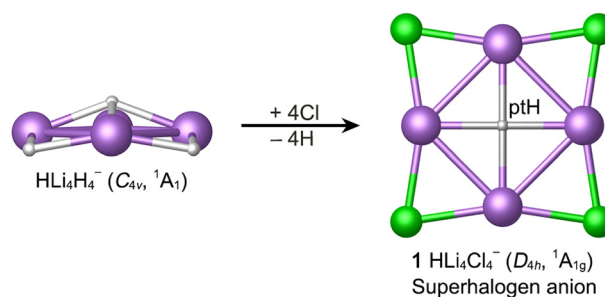
Jack M. Woolley, Natercia D. N. Rodrigues, Josene M. Toldo,\* Benjamin Rioux, Chris Groves, Xandra Schrama, Jimmy Alarcán, Temitope T. Abiola, Matthieu M. Mention, Mariana T. do Casal, Simon E. Greenough, Marise Borja, Wybren J. Buma,\* Michael N. R. Ashfold,\* Albert Braeuning,\* Teun Munnik,\* Keara A. Franklin,\* Florent Allais,\* Mario Barbatti and Vasilios G. Stavros\*



7383

### $\text{HLi}_4\text{Cl}_4^-$ : a planar tetracoordinate hydrogen superhalogen anion

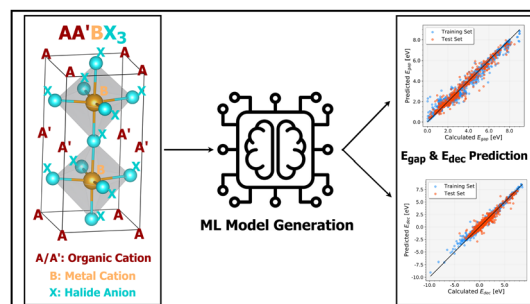
Hui-Feng Yan and Jin-Chang Guo\*



7389

### Discovering novel lead-free mixed cation hybrid halide perovskites via machine learning

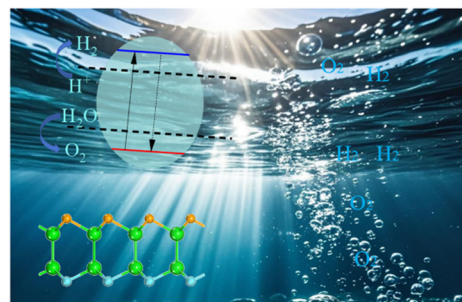
Fatemeh Jamalabijan, Somayyeh Alidoust, Gözde İniş Demir and Adem Tekin\*



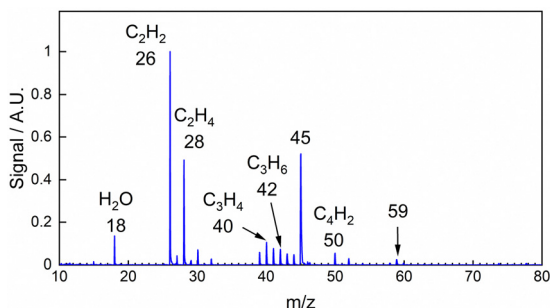
7399

### Two-dimensional Janus $\text{X}_2\text{SSe}$ ( $\text{X} = \text{Al}, \text{Ga}$ or $\text{In}$ ) monolayers: potential photocatalysts with low effective mass

Jinyi Zhu, Xinguo Ma,\* Tian Xie, Yijing Ren and Yujin Liu



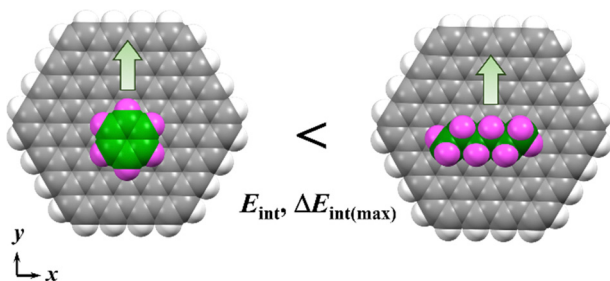
7409



### Experimental studies of high-temperature thermal dissociation of iso-propanol

John H. Kim,\* Keunsoo Kim, Qinghui Meng, Ashish Sutar, Margaret S. Wooldridge and Robert S. Tranter

7421

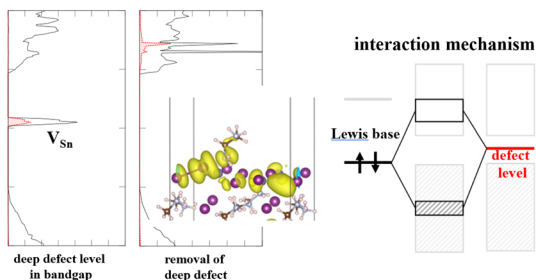


### Stability of polycyclic aromatic hydrocarbons on graphite: resistance to horizontal displacement

Yoshihiro Kikkawa\* and Seiji Tsuzuki\*

7429

### molecular passivation for Sn-Ge-mixed perovskite

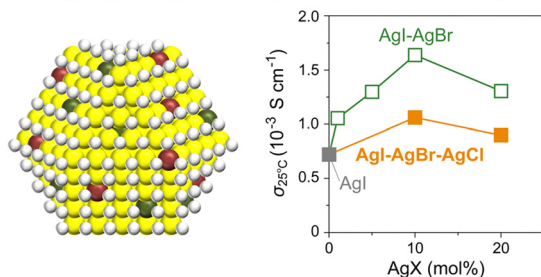


### A theoretical study of the molecular passivation of p-/n-type defects on tin- and germanium-mixed perovskite surfaces using Lewis base/acid

Emi Kino, Makito Takagi,\* Takumi Naito, Masanori Tachikawa, Koichi Yamashita and Tomomi Shimazaki\*

7440

### AgI-AgBr-AgCl / Mesoporous alumina (MPA)



### Systematic study of ionic conduction in silver iodide/mesoporous alumina composites 3: effects of binary silver halide doping

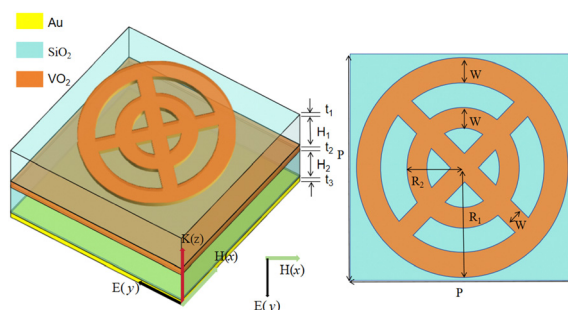
Yoko Fukui,\* Yukihiko Yoshida,\* Hiroshi Kitagawa and Yohei Jikihara



7447

### Tunable ultra-broadband plasmonic terahertz absorber based on ultrathin phase-change metamaterials

Dian Wang, Wei Wang, Yilin Jia, Huihui Cheng, Xinran Ji, Haoru Zhang\* and Qiannan Wu\*



7456

### Impact of mass transport on meniscus electrochemistry determined by time-resolved *operando* X-ray photoelectron spectroscopy

Alenka Križan, Tove Ericson, Laura King, Qianhui Liu, Robert Temperton, Robert Dominko, Ožbej Vodeb, Dušan Strmčnik, Miran Gaberšček\* and Maria Hahlin\*

