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#### Inside cover

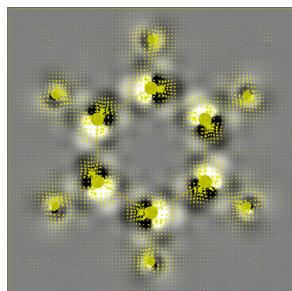
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### COMMUNICATIONS

6832

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

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

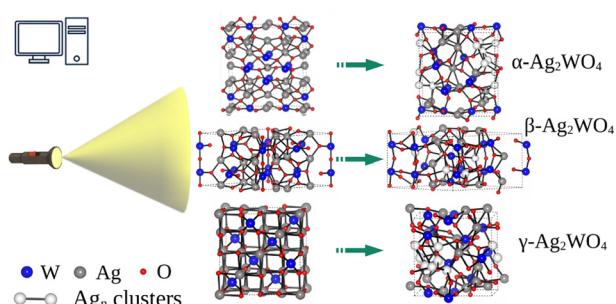


$$\tilde{\mathbf{J}} - \tilde{\mathbf{j}} = \frac{\nabla}{4\pi} \int \frac{\nabla' \cdot \tilde{\mathbf{j}}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}'$$

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#### 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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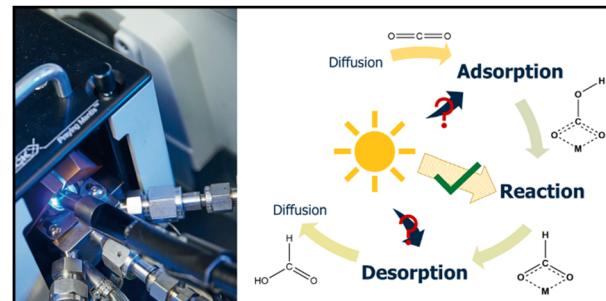
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## COMMUNICATIONS

6845

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

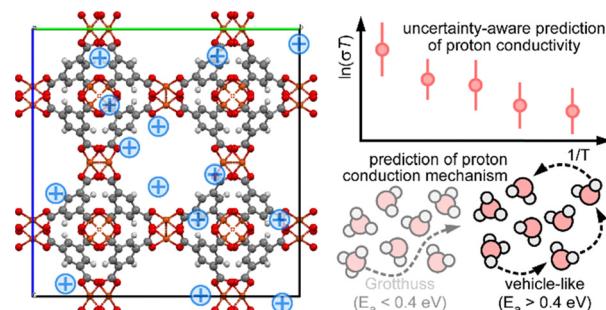
Pawel Naliwajko, Nikolaos G. Moustakas, Marcus Klahn, Tim Peppel and Jennifer Strunk\*



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**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

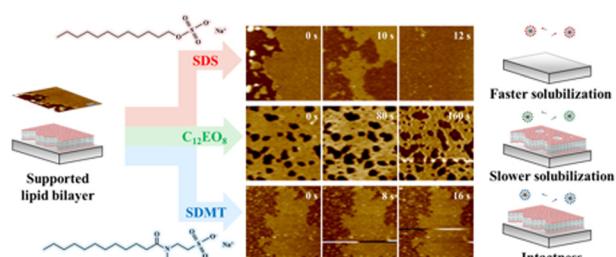


## RESEARCH PAPERS

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

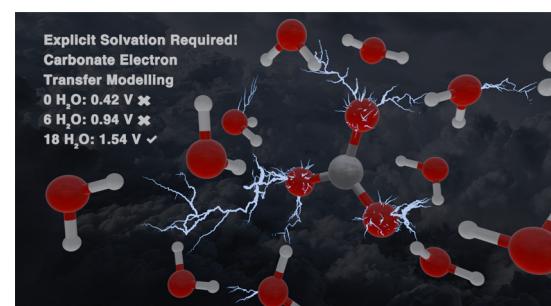
Masaki Hanzawa,\* Hiroaki Sugasawa, Taku Ogura, Ken-ichi Iimura\* and Takeshi Misono



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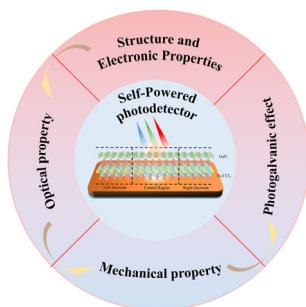
**Role of explicit solvation and level of theory in predicting the aqueous reduction potential of carbonate radical anion by DFT**

Michael R. Dooley and Shubham Vyas\*



## RESEARCH PAPERS

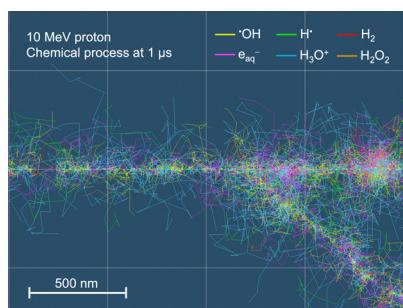
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Guoqing Zhang, Zhen Cui,\* Aming Song, Shuang Zhang and Lu Wang

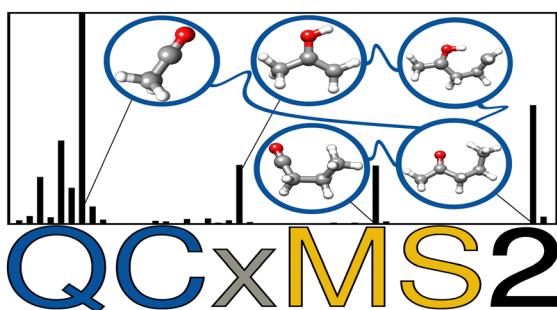
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## Development of a chemical code applicable to ions based on the PHITS code for efficient and visual radiolysis simulations

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

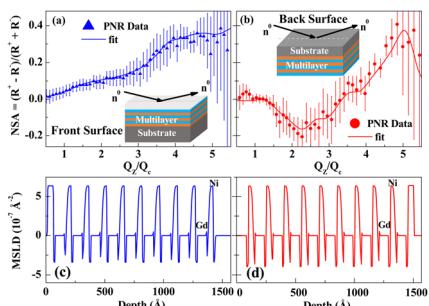
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## QCxMS2 – a program for the calculation of electron ionization mass spectra via automated reaction network discovery

Johannes Gorges and Stefan Grimme\*

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

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

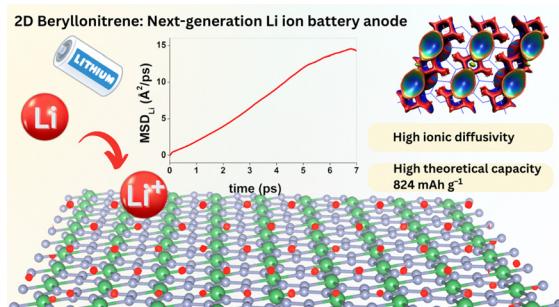


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**Exploring the potential of 2D beryllonitrene as a lithium-ion battery anode: a theoretical study**

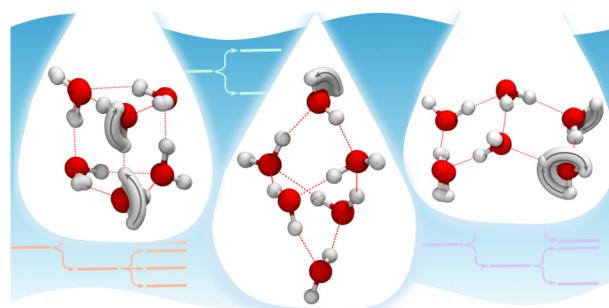
Antara Vaidyanathan, Harkishan Dua, Utpal Sarkar, Nicola Seriani\* and Brahmananda Chakraborty\*



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

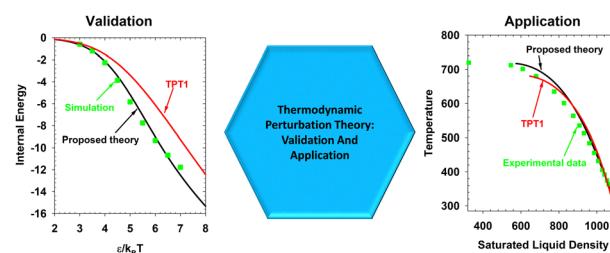
Nina Tokić, Mihael Eraković and Marko T. Cvitaš\*



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

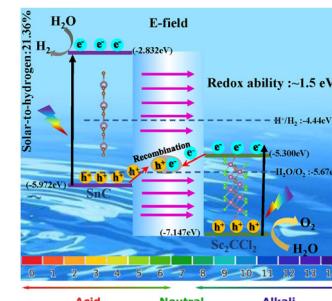
Mahmood Abdi and Hassan Hassanzadeh\*



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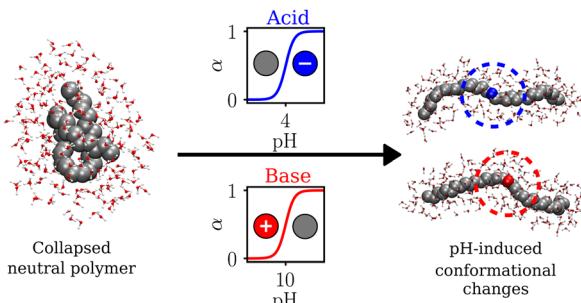
**Z-Scheme heterostructures of 2D SnC/Sc<sub>2</sub>CCl<sub>2</sub> for overall water splitting with strong redox potential under visible light**

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



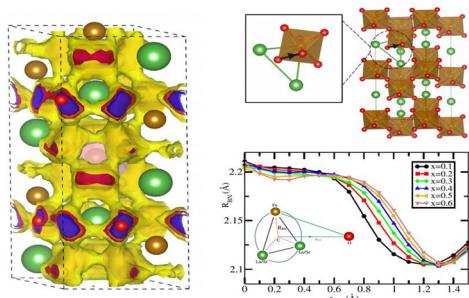
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**A generic model for pH-sensitive collapse of hydrophobic polymers**

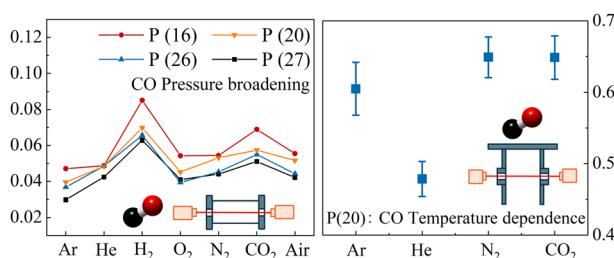
Varun Mandalaparthy\* and Nico F. A. van der Vegt

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**Molecular dynamics studies of oxide ion transport in Sr-doped  $\text{LaFeO}_3$ : role of cationic environments and cooperativity**

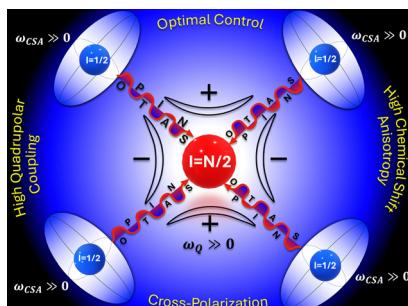
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**Measurement of carbon monoxide pressure broadening and temperature dependence coefficients in the  $1 \leftarrow 0$  band**

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

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

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

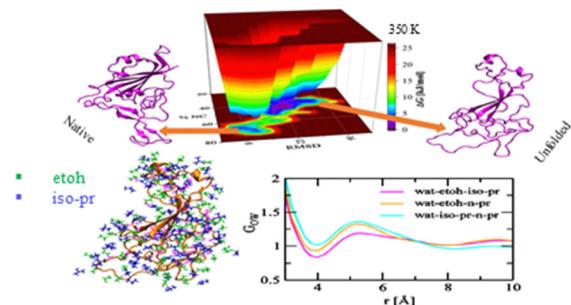


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**Unraveling the impact of binary vs. ternary alcohol solutions on the conformation and solvation of the SARS-CoV-2 receptor-binding domain**

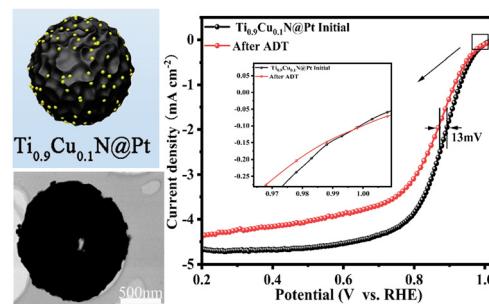
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**Designed synthesis of multi-defective  $\text{Ti}_{0.9}\text{Cu}_{0.1}\text{N}@\text{Pt}$  as a robust catalyst for the oxygen reduction reaction**

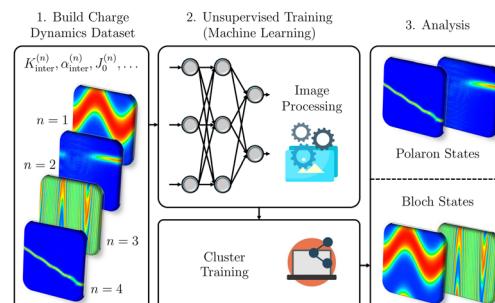
Sipeng Chen, Jiquan Lu, Yuying Li,  
Yuying Zheng\* and Ting Zhu\*



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

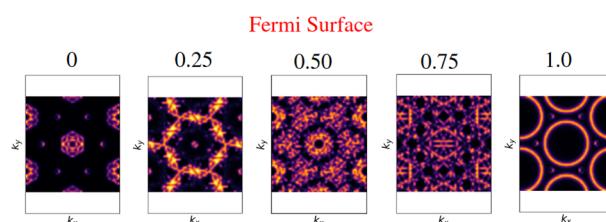
T. S. A. Cassiano, M. L. Pereira Junior,  
P. H. de Oliveira Neto\* and L. A. Ribeiro Junior



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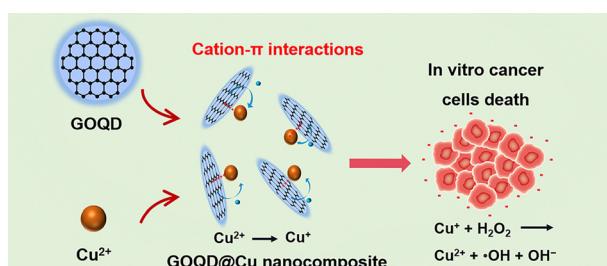
**The influence of interlayer bias and crystal field on the electronic characteristics of twisted tri-layer graphene**

Mufasila Mumthaz Muhammed and  
Junais Habeeb Mokkath\*



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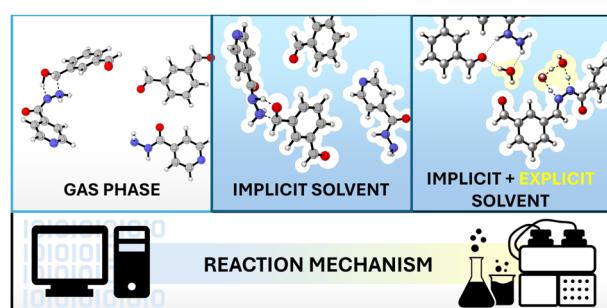
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### Enhanced anticancer activity of graphene oxide quantum dot@Cu nanocomposites via cation- $\pi$ interactions

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

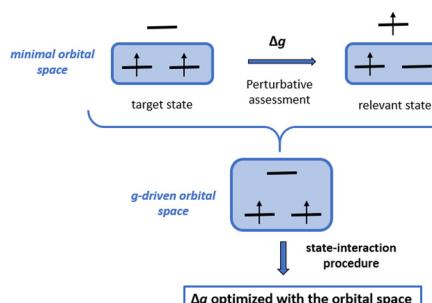
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### Mechanistic insights on hydrazones synthesis: a combined theoretical and experimental study

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

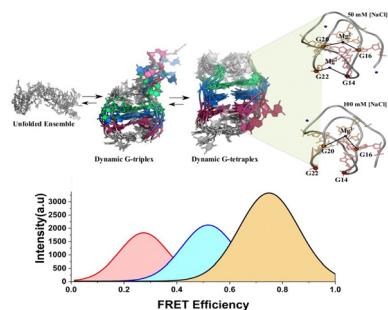
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### Efficient state-interaction approach for the g-matrix analysis in high-spin molecules

Antonio Cebreiro-Gallardo and David Casanova\*

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### 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\*

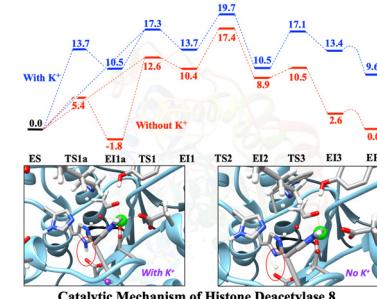


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**Deacetylation mechanism of histone deacetylase 8: insights from QM/MM MP2 calculations**

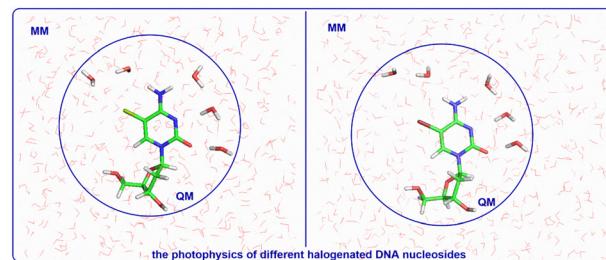
Rui Lai\* and Hui Li\*



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**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**

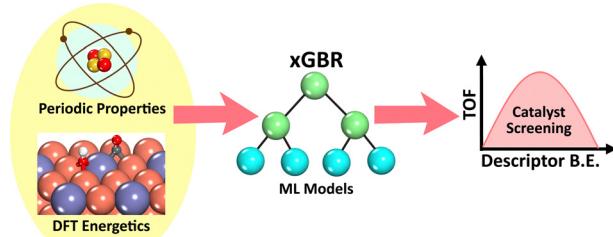
Xue-Ping Chang,\* Feng-Ran Fan, Ke Liu, Hai-Ting Lv, Geng Zhao, Lingyun Zheng, Teng-Shuo Zhang and Bin-Bin Xie



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

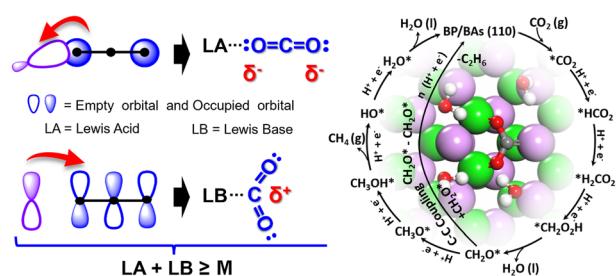
Pallavi Dandekar, Aditya Singh Ambesh, Tuhin Suwra Khan and Shelaka Gupta\*



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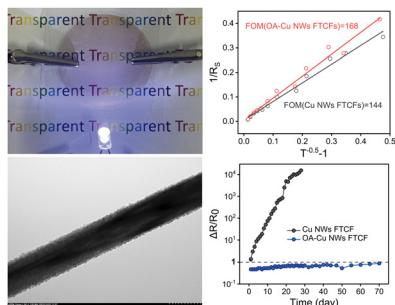
**Tailoring frustrated Lewis pair catalysts for enhanced electrochemical CO<sub>2</sub> reduction to multi-carbon fuels**

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



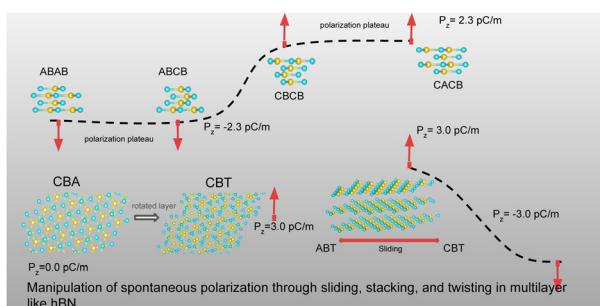
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**High initial conductivity and oxidation resistance of copper nanowire films via depositing oxalic acid**

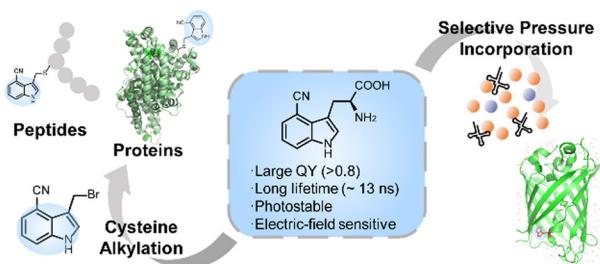
Weiqiang Yuan, Xingzhong Zhu,\* Jizhe Zhang, Juan Xu, Yuhao Zhang, Junyao Cai, Ning Peng and Caixia Kan\*

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**Slide and twist: manipulating polarization in multilayer hexagonal boron–nitride**

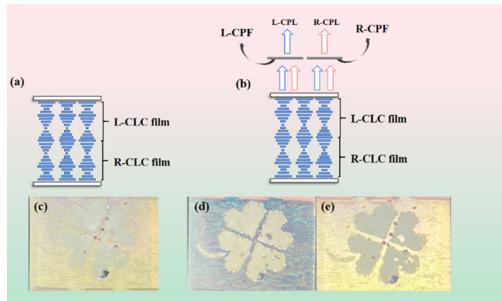
Sanber Vizcaya,\* Felipe Pérez Riffó, Juan M. Florez and Eric Suárez Morell

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**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\*

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

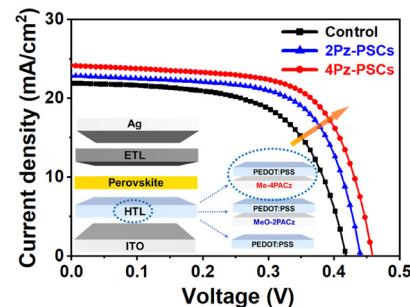


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**Interface modification of hole transport layers in tin-based halide perovskite solar cells**

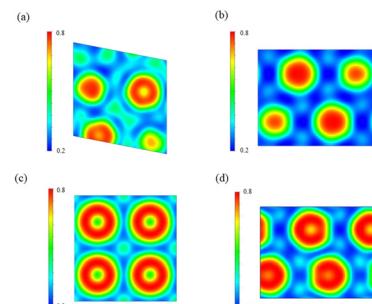
Xin Zhang, Xinyao Chen, Zhenjun Li, Jin Cheng,  
Chunqian Zhang and Junming Li\*



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

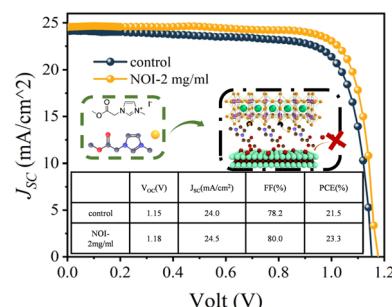
Xiaoshang Wen, Runqing Zhang, Junzhao Li,  
Jingyi Zhang, Haijie Zhang, Huafeng Dong,\*  
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**Multifunctional small molecule interface management for efficient planar perovskite solar cells**

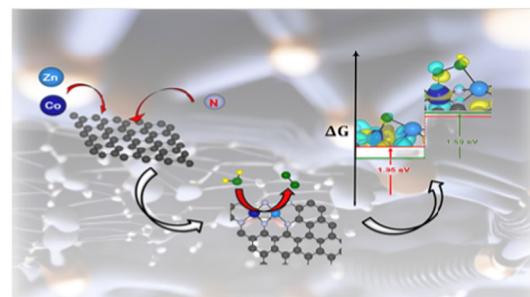
Rui Zhou, Xin Hu, Haijin Li, Huiyao Zhao, Yanbei Wei,  
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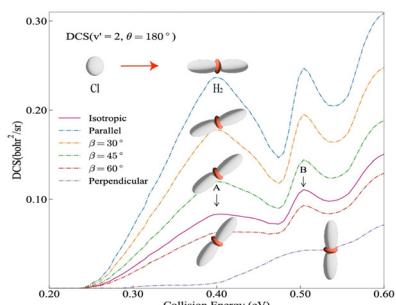
**Deciphering the impact of Zn-incorporation on M-NC (M = Fe, Co, Ni, Cu) type catalysts for enhanced HER and OER performance**

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



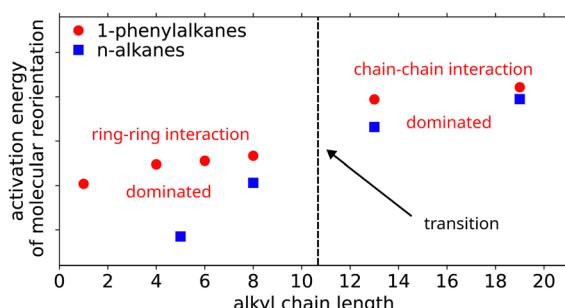
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**Stereodynamical control of resonances in the  $\text{Cl} + \text{H}_2$  ( $v = 1, j = 1$ )  $\rightarrow \text{HCl} + \text{H}$  reaction**

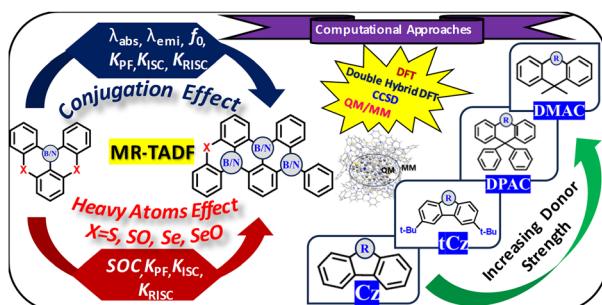
Xiaoxi Xu, Bayaer Buren\* and Maodu Chen\*

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

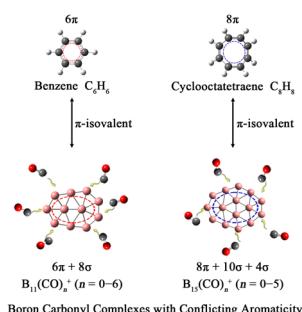
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**A theoretical investigation of heavy atom and oxidation effects in MR-TADF emitters for OLEDs: a combined DFT, double hybrid DFT, CCSD, and QM/MM approaches**

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

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

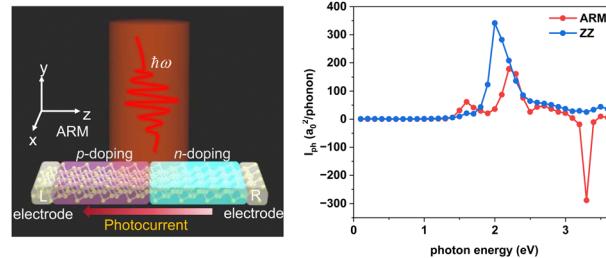


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**First-principles analysis of the photocurrent in a monolayer  $\alpha$ -selenium p–n junction optoelectronic device**

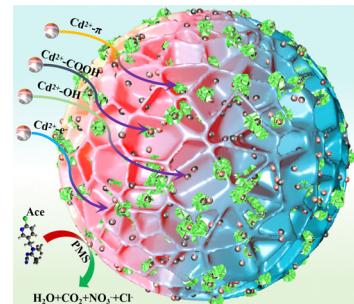
Yujian Wang, Xiaoyong Xiong, Shibo Fang, Hong Li, Zhiulin Weng, Dahua Ren and Qiang Li\*



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

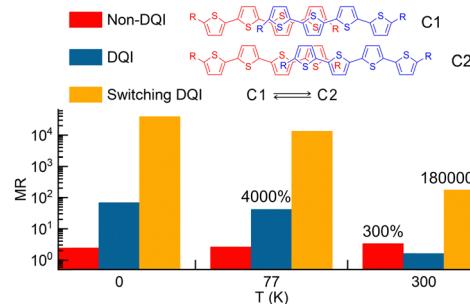
Xiaojuan Su, Pengfei Gao, Yuanchuan Ren,\* Jieba Li and Nanqi Ren\*



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**Molecular magnetoresistance enhanced by destructive quantum interference of a  $[\pi \cdots \pi]$  supramolecule**

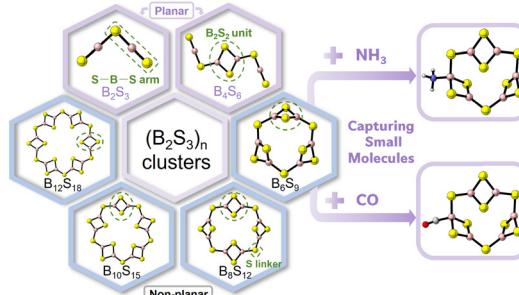
Hua Hao,\* Shuhui Qin, Ting Jia\* and Xiaohong Zheng



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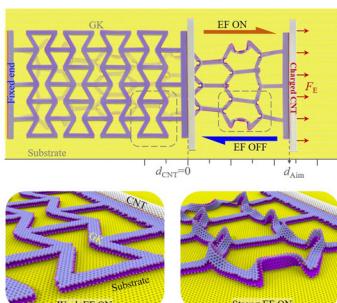
**Structural evolution and electronic properties of boron sulfides  $(\text{B}_2\text{S}_3)_n$  ( $n = 1\text{--}6$ ): insights from DFT calculations**

Jingxin Hu, Lin Zhang and Zexing Cao\*



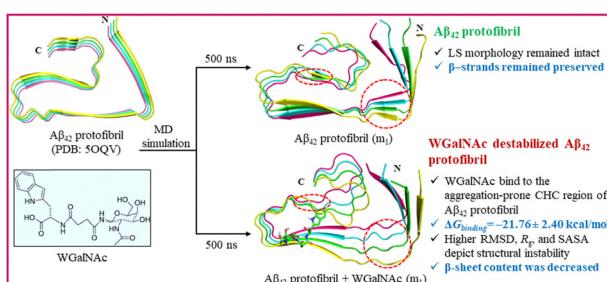
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**A high-frequency nanoscale positioner driven by an external electric field: a molecular dynamics study**

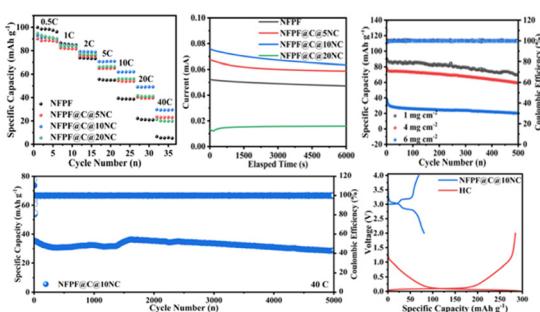
Huichang Feng, Kun Cai,\* Jiao Shi and Yingyan Zhang\*

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

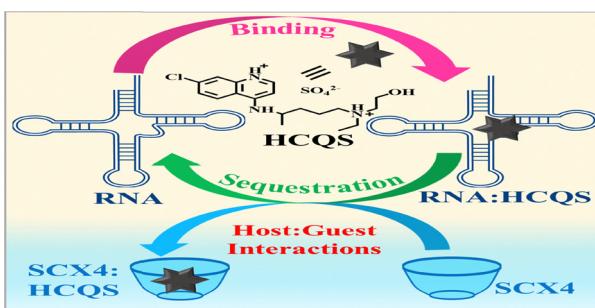
Arushi Dabas and Bhupesh Goyal\*

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**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\*

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**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\*

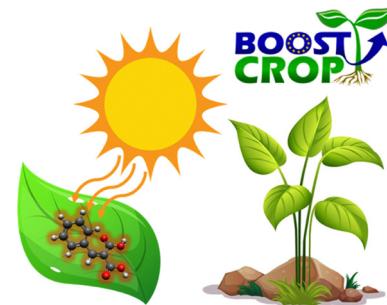


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**Molecular heaters: a green route to boosting crop yields?**

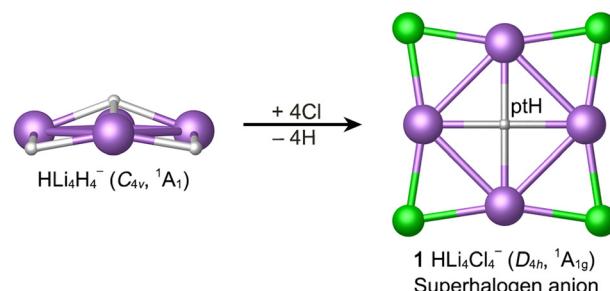
Jack M. Woolley, Natercia D. N. Rodrigues,  
 Josene M. Toldo,\* Benjamin Rioux, Chris Groves,  
 Xandra Schrama, Jimmy Alarcan, Temitope T. Abiola,  
 Matthieu M. Mention, Mariana T. do Casal,  
 Simon E. Greenough, Marise Borja, Wybren J. Buma,\*  
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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



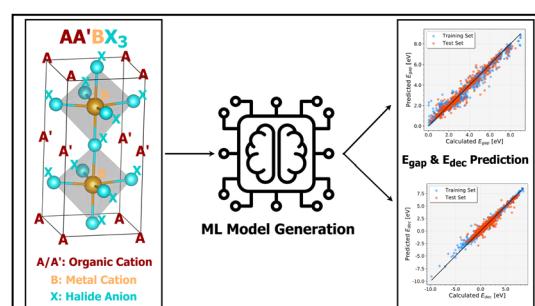
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Hui-Feng Yan and Jin-Chang Guo\*



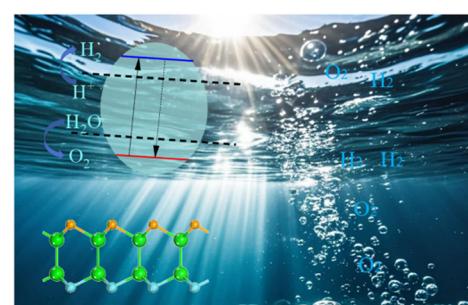
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 Gözde İniş Demir and Adem Tekin\*

7399

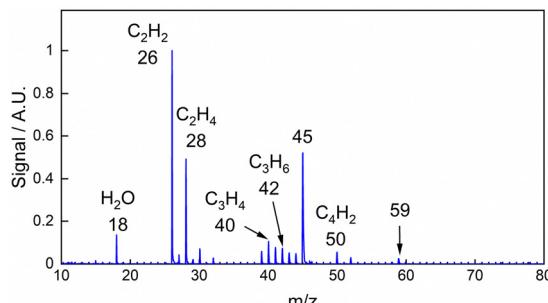
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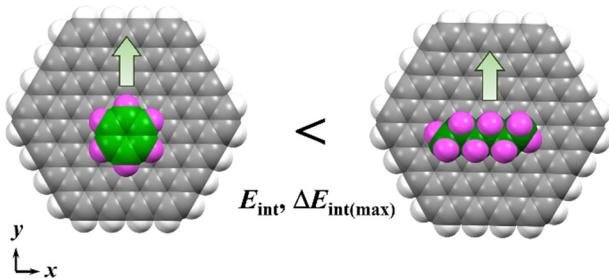
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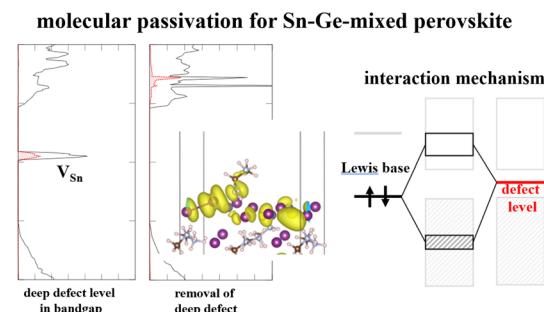
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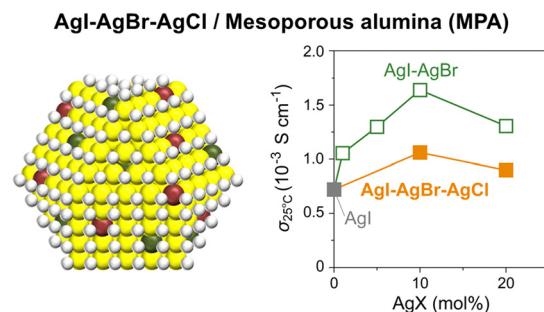
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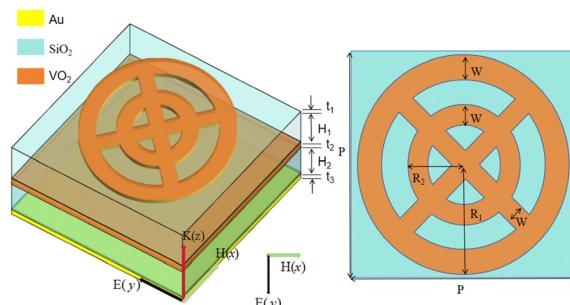


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