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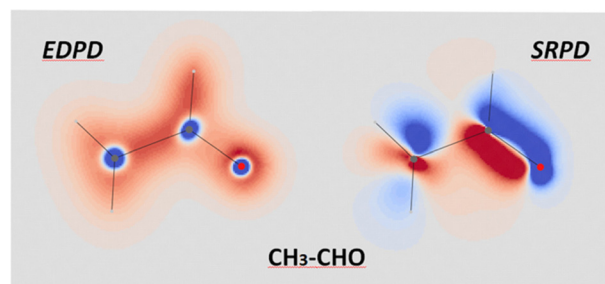
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*Phys. Chem. Chem. Phys.*,  
2023, **25**, 25094.

## PERSPECTIVE

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### Electronic current densities and origin-independent property densities induced by optical fields

Francesco F. Summa, Guglielmo Monaco,  
Paolo Lazzeretti and Riccardo Zanasi\*

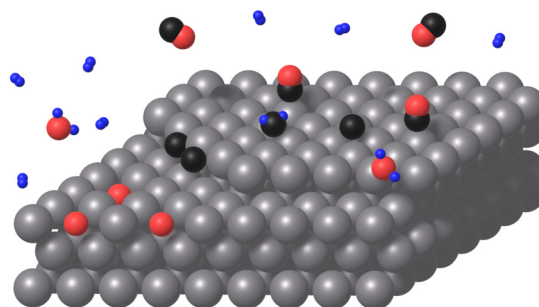


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### Spectroscopic investigation of a Co(0001) model catalyst during exposure to H<sub>2</sub> and CO at near-ambient pressures

Sabine Wenzel, Dajo Boden, Richard van Lent,  
Elahe Motaee, Mahesh K. Prabhu, Hamed Achour and  
Irene M. N. Groot\*



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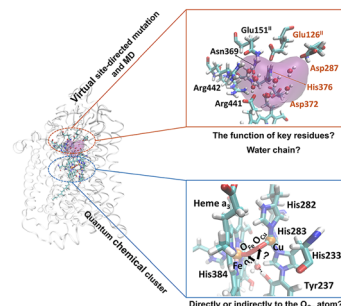


## RESEARCH PAPERS

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### New insights into the proton pumping mechanism of $\text{ba}_3$ cytochrome *c* oxidase: the functions of key residues and water

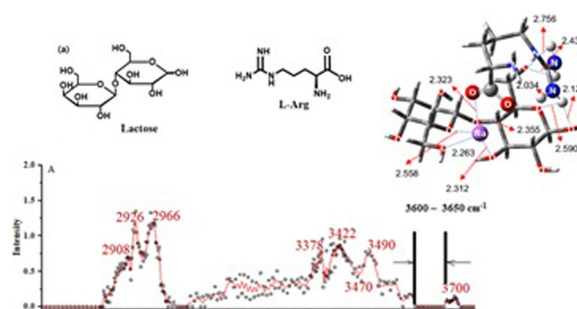
Xiaoyue Yang, Shaohui Liu, Zhili Yin, Mengguo Chen, Jinshuai Song, Pengfei Li and Longhua Yang\*



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### Distinguishing gas phase lactose and lactulose complexed with sodiated L-arginine by IRMPD spectroscopy and DFT calculations

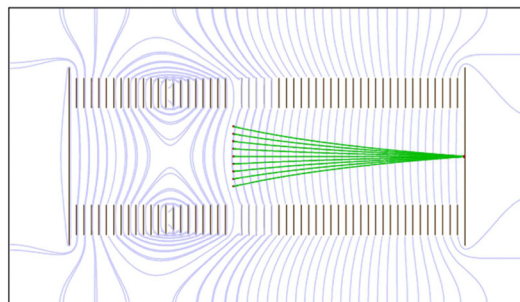
Min Kou, Young-Ho Oh, Sungyul Lee\* and Xianglei Kong\*



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### Velocity map imaging with no spherical aberrations

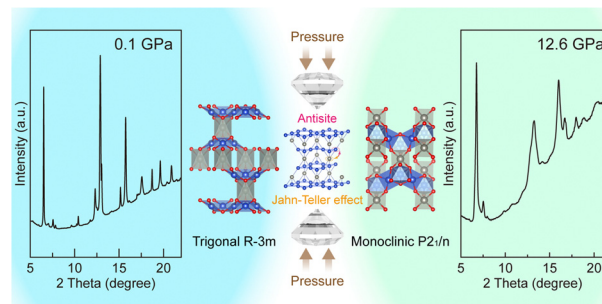
Yehuda Ben-Shabo, Adeliya Kurbanov, Claus Dieter Schröter, Robert Moshhammer, Holger Kreckel and Yoni Toker\*



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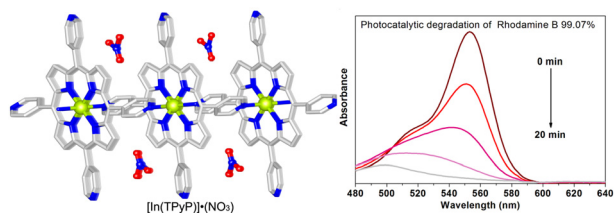
### Structural phase transformation of quantum spin liquid herbertsmithite *via* pressure induced enhancement of the cooperative Jahn–Teller effect and antisite disorder

Yaxiao Luo, Jian Zhang,\* Jiayi Wu, Hui Tian, Yanmei Ma, Lina Jiang, Hang Cui and Qiliang Cui



## RESEARCH PAPERS

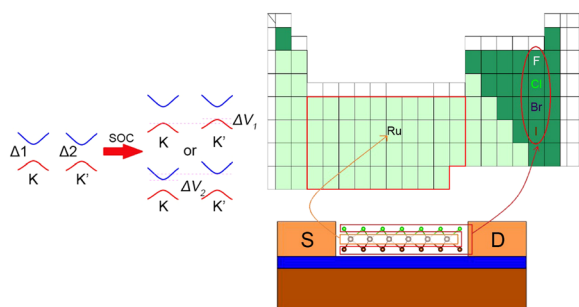
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### Fast photocatalytic degradation of rhodamine B using indium-porphyrin based cationic MOF under visible light irradiation

Chang-Xun Dou, Xu-Ke Tian, Ying-Jun Chen, Pei-Pei Yin, Jia-Hui Guo, Xiao-Gang Yang,\* Yu-Ming Guo\* and Lu-Fang Ma

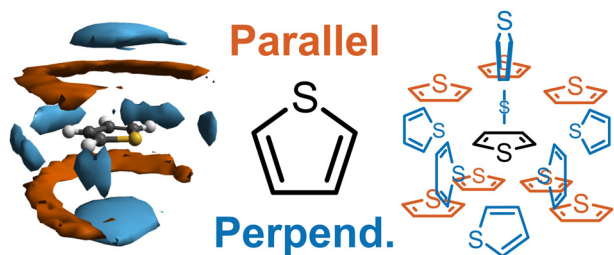
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### Two dimensional Janus RuXY (X, Y = Br, Cl, F, I, X ≠ Y) monolayers: ferromagnetic semiconductors with spontaneous valley polarization and tunable magnetic anisotropy

Ziyu Liu, Baozeng Zhou, Xiaocha Wang\* and Wenbo Mi\*

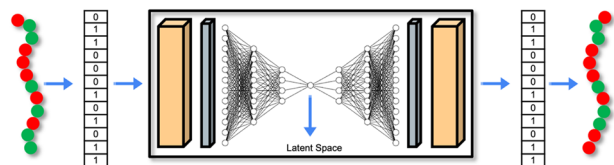
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### The structure of liquid thiophene from total neutron scattering

Thomas F Headen,\* Camilla Di Mino, Tristan GA Youngs and Adam J Clancy\*

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### Developing efficient deep learning model for predicting copolymer properties

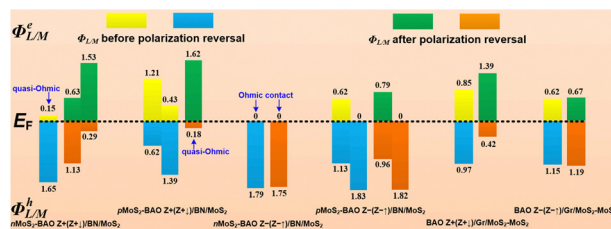
Himanshu, Kaushik Chakraborty and Tarak K. Patra\*



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### Polarization-tunable interfacial properties in monolayer-MoS<sub>2</sub> transistors integrated with ferroelectric BiAlO<sub>3</sub>(0001) polar surfaces

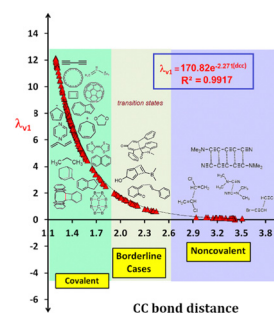
Jin Yuan, Jian-Qing Dai,\* Yu-Zhu Liu and Miao-Wei Zhao



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### Topology of electrostatic potential and electron density reveals a covalent to non-covalent carbon-carbon bond continuum

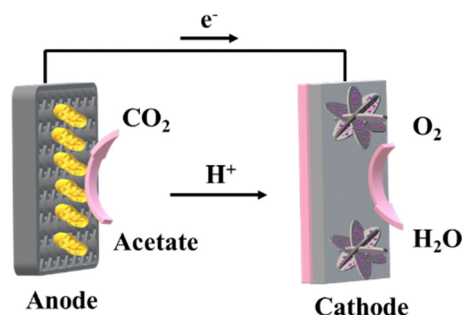
Puthannur K. Anjalikrishna, Shridhar R. Gadre\* and Cherumuttathu H. Suresh\*



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### High power density output and durability of microbial fuel cells enabled by dispersed cobalt nanoparticles on nitrogen-doped carbon as the cathode electrocatalyst

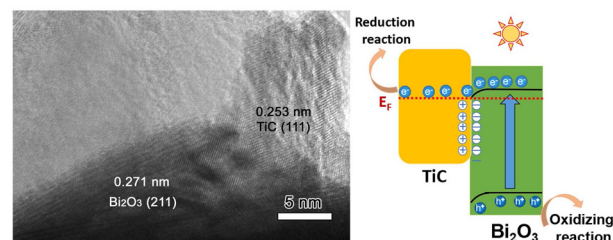
Yuxian Yang, Jialuo Lin, Xin Li, Zhuoyue Chen, Yingyu Lin, Mengqing Xu and Weishan Li\*



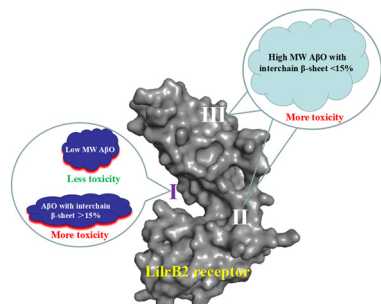
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### Non-noble-metal TiC-nanoparticle-promoted charge separation and photocatalytic degradation performance on Bi<sub>2</sub>O<sub>3</sub> microrods: degradation pathway and mechanism investigation

Tao Xian,\* Ke Ma, Lijing Di,\* Xuelian Ma, Xiaofeng Sun and Hua Yang



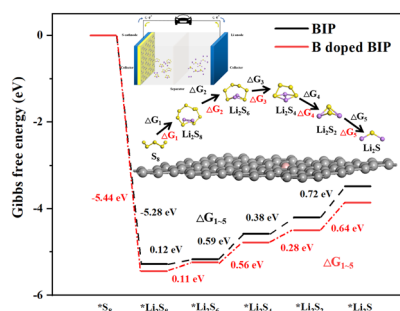
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### Identification and characterization of the conformation and size of amyloid- $\beta$ (42) oligomers targeting the receptor LILRB2

Jinfei Mei, Wen Xu, Wenqi Gao, Chuanbo Wang, Yvning Guan, Sajjad Ahmad and Hongqi Ai\*

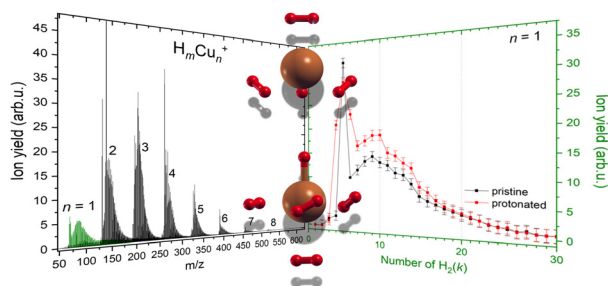
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### Theoretical prediction of 2D biphenylene as a potential anchoring material for lithium-sulfur batteries

Han Wang, Fan Kong, Zonggang Qiu, Jiyuan Guo,\* Huabing Shu and Qin Wei

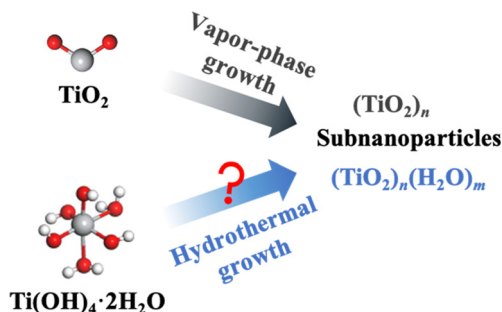
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### Solvation of cationic copper clusters in molecular hydrogen

O. V. Lushchikova,\* J. Reichegger, S. Kollotzek, F. Zappa, M. Mahmoodi-Darian, M. Bartolomei,\* J. Campos-Martínez, T. González-Lezana, F. Pirani and P. Scheier

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### Aqueous growth of titania subnanoparticles: an understanding of the ultrasmall visible-light-absorbing unit of $(\text{TiO}_2)_8(\text{H}_2\text{O})_{16}$

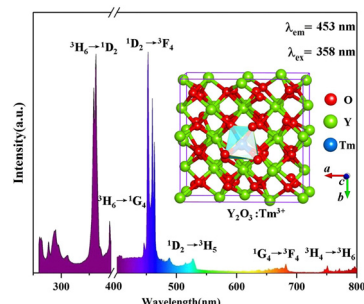
Jiawei Wu, P. Hu and Haifeng Wang\*



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### Photoluminescence and energy transfer mechanisms of $\text{Tm}^{3+}$ doped $\text{Y}_2\text{O}_3$ laser crystals: experimental and theoretical insights

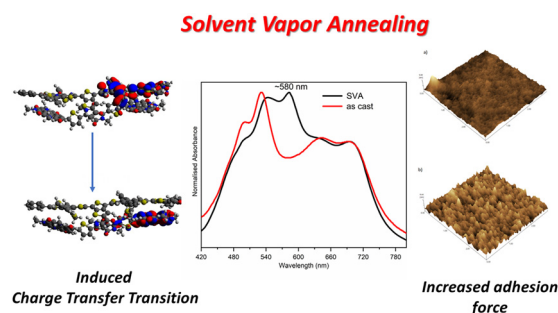
Meng Ju,\* Hongkuan Yuan, Wenhao Ji, Lei Zhao,\* Yang Xiao and Yauyuen Yeung\*



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### Effects of solvent vapor annealing on the optical properties and surface adhesion of conjugated D:A thin films

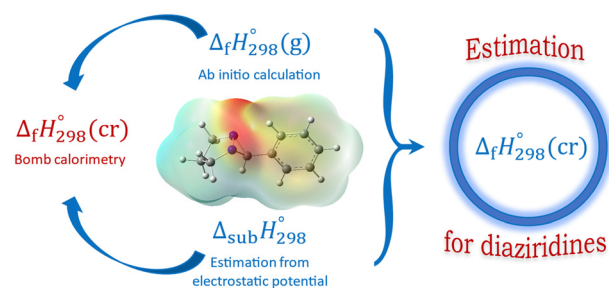
Tainã Reges Casagrande, Juscelino Valter Barbosas Júnior, Jaqueline Cristine Desordi, Mariana Richelle Pereira da Cunha, Anderson Emanuel Ximim Gavim, Luciano Nassif Vidal, Paula Cristina Rodrigues, Indrani Coondoo, Douglas J. Coutinho, Roberto Mendonça Faria and Andreia Gerniski Macedo\*



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### Enthalpy of formation of 6-phenyl-1,5-diazabicyclo[3.1.0]hexane by combustion calorimetry and theoretical approach for efficient prediction of thermochemistry of diaziridines

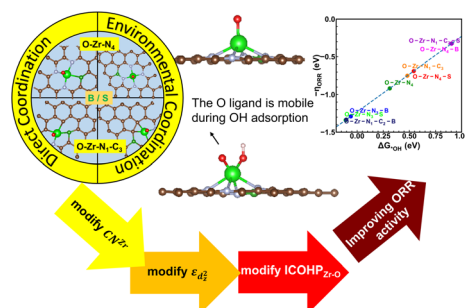
Vera A. Lukyanova, Vladimir V. Kuznetsov, Natalia M. Konstantinova, Andrey S. Dmitrenok, Maria P. Kosaya, Olga V. Dorofeeva\* and Anna I. Druzhinina



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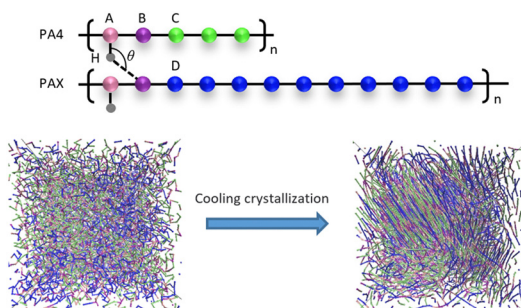
### Coordination engineering of atomically dispersed zirconium on graphene for the oxygen reduction reaction

Jessie Manopo, Pangeran Niti Kusumo, Afriyanti Sumboja and Yudi Darma\*



## RESEARCH PAPERS

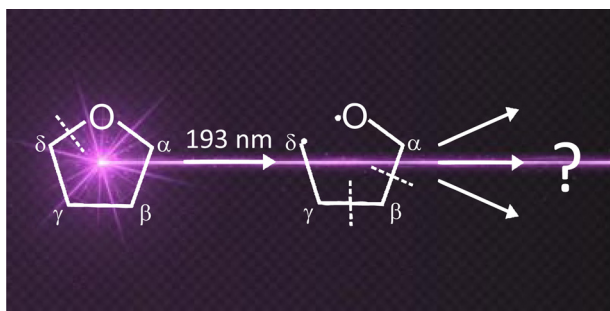
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### Molecular dynamics simulation and non-isothermal crystallization kinetics of polyamide 4 and different bio-based polyamide blends

Yajing Zhang, Mingda Wang, Liquan Wang, Tao Chen, Weisheng Feng, Tianyi Wang and Liming Zhao\*

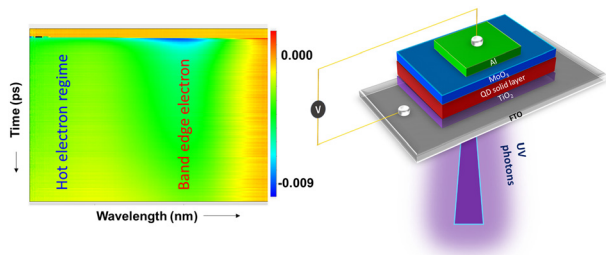
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### Photodissociation dynamics of tetrahydrofuran at 193 nm

Dennis Milešević, Joseph Stimson, Divya Popat, Patrick Robertson and Claire Vallance\*

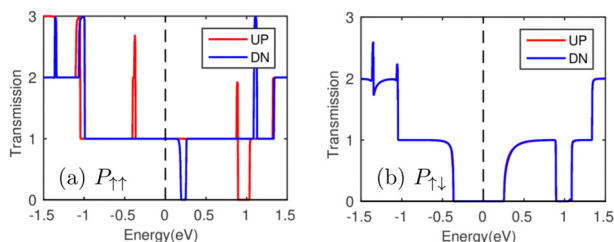
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### Induced UV photon sensing properties in narrow bandgap CdTe quantum dots through controlling hot electron dynamics

Thankappan Thrupthika, Devaraj Nataraj,\* Subramaniam Ramya, Arumugam Sangeetha and T. Daniel Thangadurai

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### Momentum matching induced giant magnetoresistance in two-dimensional magnetic tunnel junctions

Yaohua Qiu, Chun-Sheng Liu, Xingqiang Shi, Xiaohong Zheng\* and Lei Zhang\*



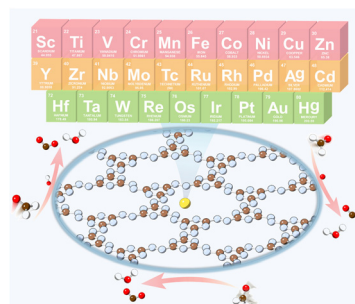


## RESEARCH PAPERS

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### Efficient degradation of formaldehyde based on DFT-screened metal-doped $C_3N_6$ monolayer photocatalysts: performance evaluation and mechanistic insights

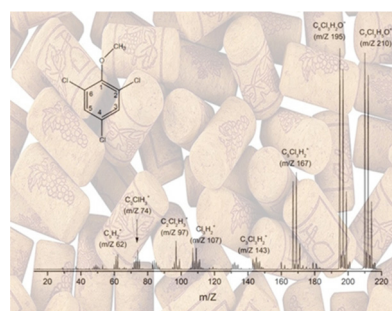
Mengshan Chen, Haijian Wang, Jinhu Wang, Mingyuzhi Sun, Yaxuan Hu, Xue Zhao\* and Yingtang Zhou\*



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### Electron ionization induced fragmentation pathways of trichloroanisole

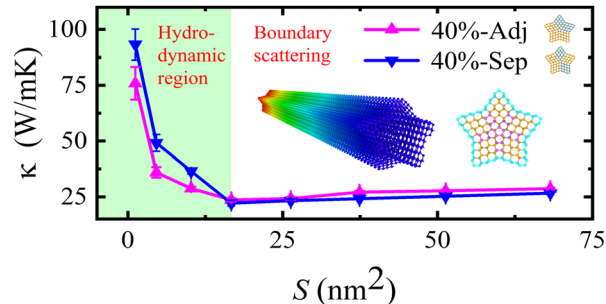
Mónica Mendes, Daniel Bou-Debes, Samuel Eden, Nenad Bundaleski, Orlando M. N. D. Teodoro, Lucas M. Cornetta\* and Filipe Ferreira da Silva\*



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### Thermal conductivity of fivefold twinned silicon-germanium heteronanowires

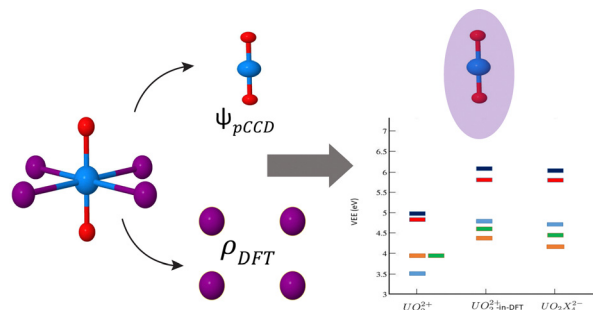
Ziyue Zhou, Jincheng Zeng, Zixuan Song, Yanwen Lin, Qiao Shi, Yongchao Hao, Yuequn Fu,\* Zhisen Zhang\* and Jianyang Wu\*



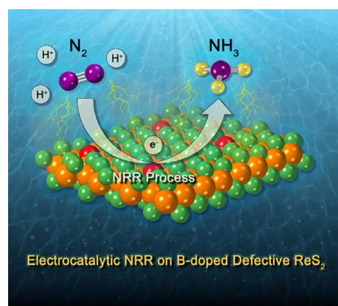
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### Static embedding with pair coupled cluster doubles based methods

Rahul Chakraborty, Katharina Boguslawski and Paweł Tecmer\*



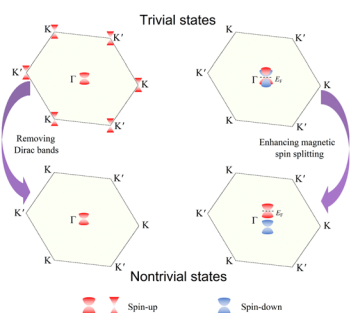
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### Unleashing the power of boron: enhancing nitrogen reduction reaction through defective ReS<sub>2</sub> monolayers

Thi H. Ho, Viet Q. Bui,\* Quynh Anh T. Nguyen, Yoshiyuki Kawazoe, Seong-Gon Kim and Pham Cam Nam

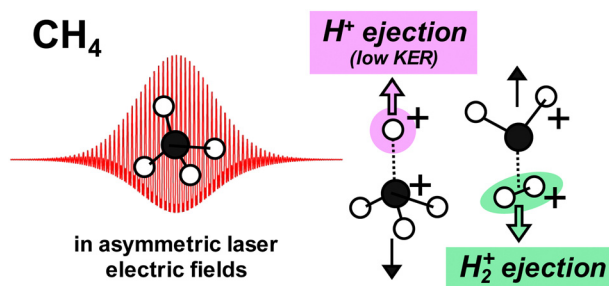
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### Engineering topological states in a two-dimensional honeycomb lattice

Yaling Zhang, Jingjing Zhang, Wenjia Yang, Huisheng Zhang\* and Jianfeng Jia\*

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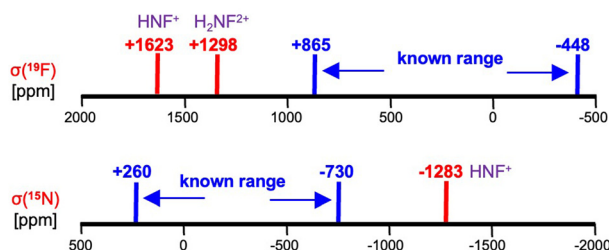


### Dissociative ionization and Coulomb explosion of CH<sub>4</sub> in two-color asymmetric intense laser fields

H. Hasegawa, A. Matsuda, T. Morishita, L. B. Madsen, F. Jensen, O. I. Tolstikhin and A. Hishikawa\*

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### Extreme NMR shielding in fluoro-nitrogen cations



### Extreme NMR shielding in fluoro-nitrogen cations

David J. D. Wilson

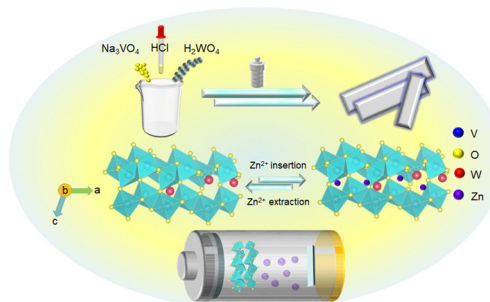


## RESEARCH PAPERS

25435

**W-doped VO<sub>2</sub> for high-performance aqueous Zn-ion batteries**

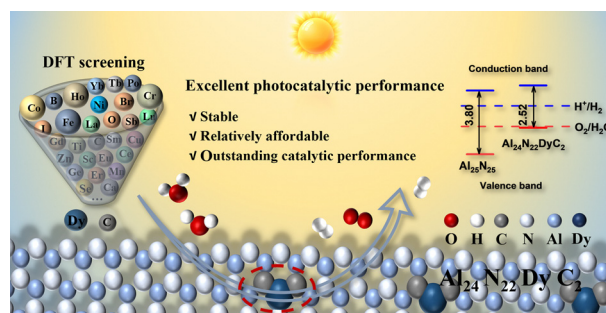
Guangxu Yang, Shuhua Yang,\* Jinfeng Sun, Guangbin Duan,\* Bingqiang Cao and Zongming Liu\*



25442

**Enhancing the photocatalytic efficiency of two-dimensional aluminum nitride materials through strategic rare earth doping**

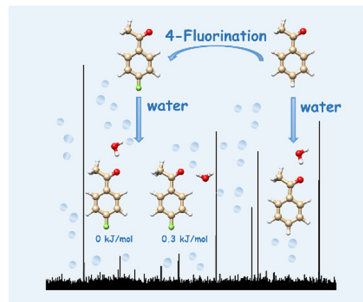
Weiyin Yan, Yayu Yan, Zirui Wang, Qiao-Hong Li\* and Jian Zhang\*



25450

**Fluorination effects probed in 4-fluoroacetophenone and its monohydrate**

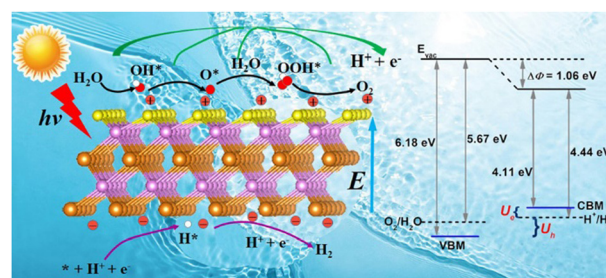
Xiujuan Wang, Jiayi Li, Juncheng Lei, Xuefang Xu,\* Yang Zheng, Junhua Chen,\* Xiao Tian and Qian Gou\*



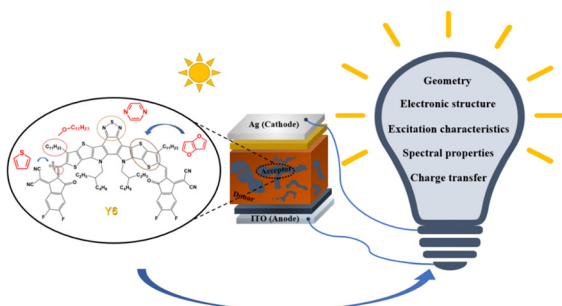
25458

**Multiple strategies of improving photocatalytic water splitting efficiency in 2D arsenic sesquichalcogenides**

Xiaoteng Li,\* Chuanlu Yang,\* Yuliang Liu, Endao Han, Wenkai Zhao, Xinxin Jiang, Dongqing Zou and Yuqing Xu



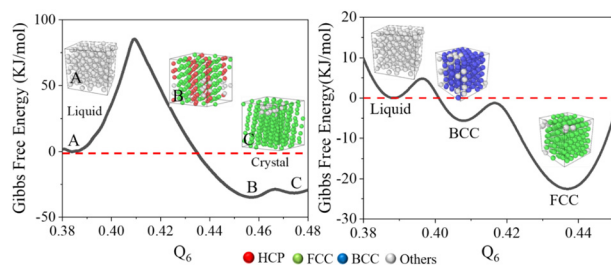
25465



### Modulating the organic photovoltaic properties of non-fullerene acceptors by molecular modification based on Y6: a theoretical study

Cai-Rong Zhang,\* Hai-Yuan Yu, Mei-Ling Zhang, Xiao-Meng Liu, Yu-Hong Chen, Zi-Jiang Liu, You-Zhi Wu and Hong-Shan Chen

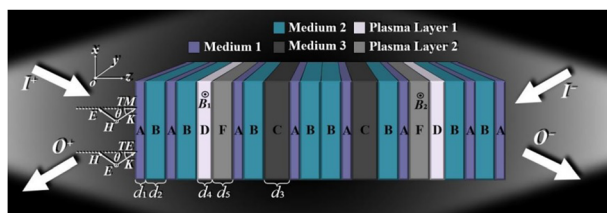
25480



### Controlling polymorph selection during nucleation by tuning the structure of metallic melts

Qi Zhang, Junjie Li, Zhijun Wang and Jincheng Wang\*

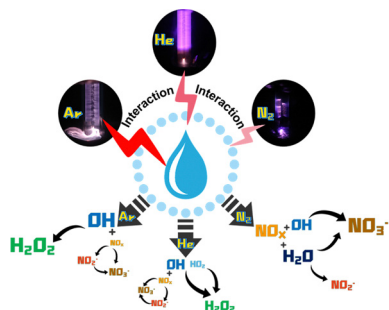
25492



### A theoretical study based on coherent perfect absorption and polarization separation in one-dimensional magnetized plasma photonic crystals

Fu Pei Wu, Jia Tao Zhang and Hai Feng Zhang\*

25499



### Repetitive pulsed gas–liquid discharge in different atmospheres: from discharge characteristics to plasma–liquid interactions

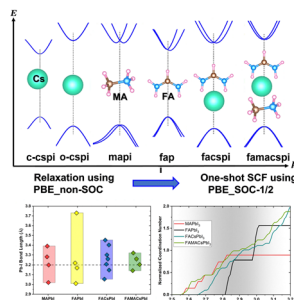
Xu Lu, Li Zhang, Sen Wang\* and Zhi Fang



25511

### Electronic and structural properties of mixed-cation hybrid perovskites studied using an efficient spin-orbit included DFT-1/2 approach

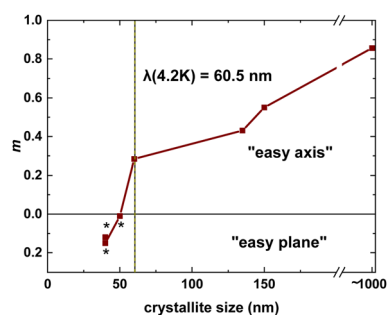
Mohammad Moaddeli, Mansour Kanani\* and Anna Grünebohm



25526

### The size effect of BiFeO<sub>3</sub> nanocrystals on the spatial spin modulated structure

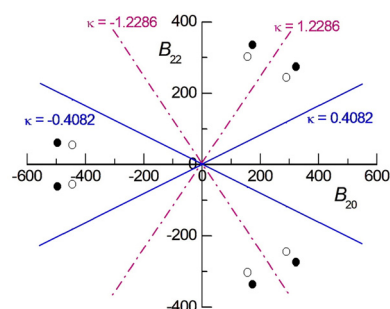
N. E. Gervits,\* A. V. Tkachev, S. V. Zhurenko, A. V. Gunbin, A. V. Bogach, N. A. Lomanova, D. P. Danilovich, I. S. Pavlov, A. L. Vasiliev and A. A. Gippius



25537

### Eu<sup>3+</sup> ions as a crystal-field probe for low-symmetry sites in doped phosphors – a case study: Eu<sup>3+</sup> at triclinic sites in Li<sub>6</sub>RE(BO<sub>3</sub>)<sub>3</sub> (RE = Y, Gd), YBO<sub>3</sub> and ZnO and at trigonal sites in YAl<sub>3</sub>(BO<sub>3</sub>)<sub>4</sub>

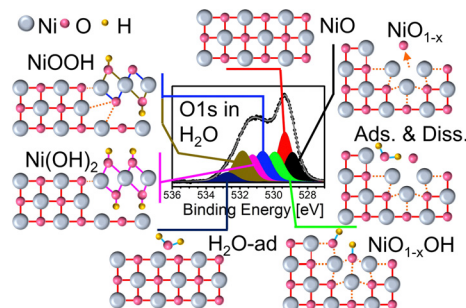
Riti Ghosh, Shankhanil Sarkar, Yatramohan Jana,\* Danuta Piwowarska, Paweł Gnutek and Czesław Rudowicz



25552

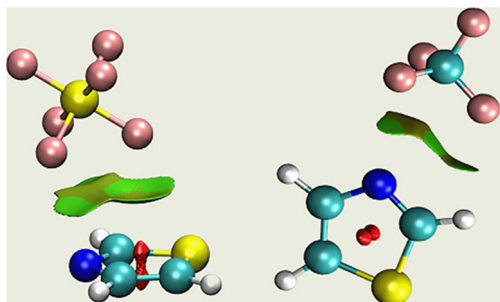
### Structural and chemical properties of NiO<sub>x</sub> thin films: the role of oxygen vacancies in NiOOH formation in a H<sub>2</sub>O atmosphere

A. Raoul Blume,\* Wolfram Calvet, Aliakbar Ghafari, Thomas Mayer, Axel Knop-Gericke and Robert Schlögl



## RESEARCH PAPERS

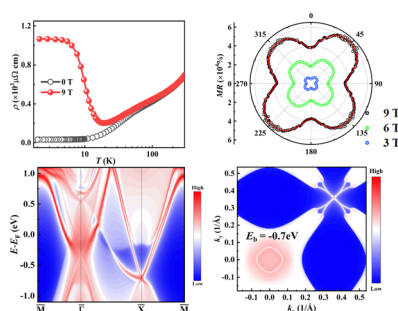
25566



### Noncovalent interactions of aromatic heterocycles: rotational spectroscopy and theoretical calculations of the thiazole–CF<sub>4</sub> and thiazole–SF<sub>6</sub> complexes

Tingting Yang, Yugao Xu, Zhen Wang, Chunmei Feng and Gang Feng\*

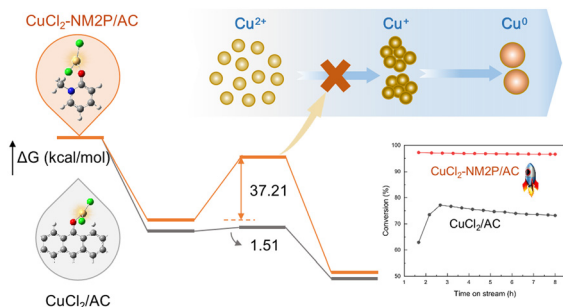
25573



### Anisotropic magnetoresistance and electronic features of the candidate topological compound praseodymium monobismuthide

F. Tang, Y. Chen, X.-L. Ge, W.-Z. Meng, Z.-D. Han, B. Qian, W. Zhao, X.-F. Jiang, Y. Fang\* and S. Ju\*

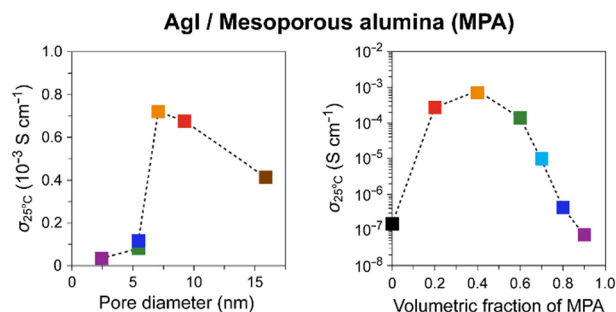
25581



### Efficient and stable N-heterocyclic ketone–Cu complex catalysts for acetylene hydrochlorination: the promotion effect of ligands revealed from DFT calculations

Yilin Zhang, Sen Li, Xianliang Qiao, Qingxin Guan\* and Wei Li\*

25594



### Systematic study of ionic conduction in silver iodide/mesoporous alumina composites 1: effects of pore size and filling level

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

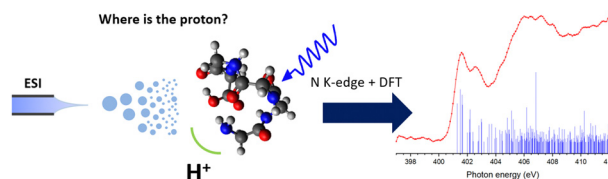


## RESEARCH PAPERS

25603

### Mapping the electronic transitions of protonation sites in peptides using soft X-ray action spectroscopy

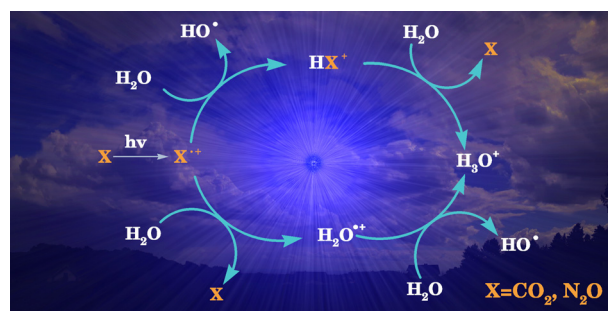
Juliette Leroux,\* Amir Kotobi, Konstantin Hirsch, Tobias Lau, Carlos Ortiz-Mahecha, Dmitrii Maksimov, Robert Meißner, Bart Oostenrijk, Mariana Rossi, Kaja Schubert, Martin Timm, Florian Trinter, Isaak Unger, Vicente Zamudio-Bayer, Lucas Schwob and Sadia Bari\*



25619

### Formation of $\text{H}_3\text{O}^+$ and $\text{OH}^-$ by $\text{CO}_2$ and $\text{N}_2\text{O}$ trace gases in the atmospheric environment

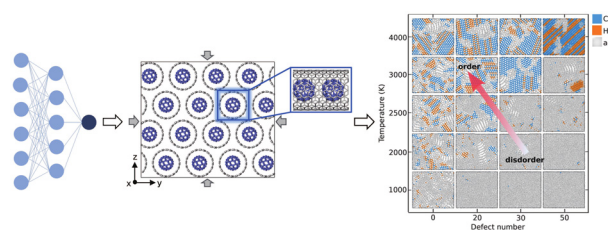
Daniele Catone, Mattea Carmen Castrovilli, Francesca Nicolanti, Mauro Satta\* and Antonella Cartoni\*



25629

### Vacancy defects impede the transition from peapods to diamond: a neuroevolution machine learning study

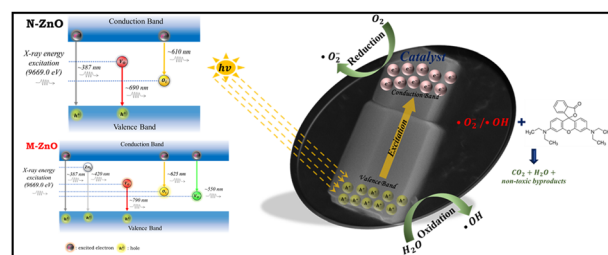
Yu Li and Jin-Wu Jiang\*



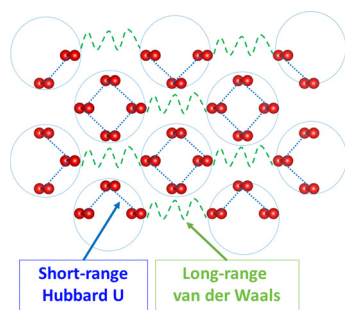
25639

### Probing size-dependent defects in zinc oxide using synchrotron techniques: impact on photocatalytic efficiency

Ankit Kadian,\* V. Manikandan, Kapil Dev, Vishnu Kumar, Cheng-Jie Yang, Bi-Hsuan Lin, C. L. Chen, C. L. Dong, K. Asokan and S. Annapoorni\*



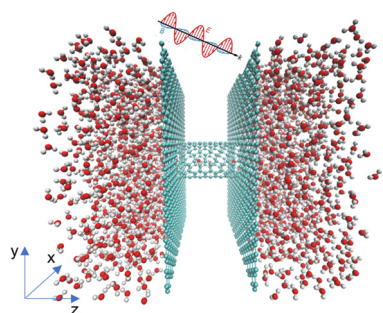
25654



### The impact of Hubbard and van der Waals corrections on the DFT calculation of epsilon–zeta transition pressure in solid oxygen

Le The Anh

25659

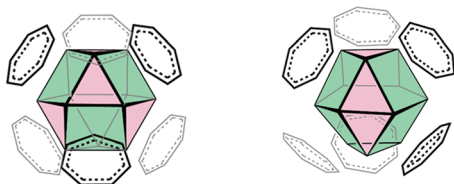


### Effect of terahertz electromagnetic field on single-file water transport through a carbon nanotube

Yunzhen Zhao,\* Keda Yang and Jiaye Su\*

25670

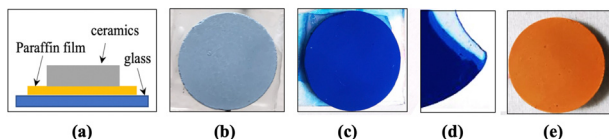
### Pd<sub>13</sub> Core: Cuboctahedral vs Anti-cuboctahedral



### Palladium cluster complex [Pd<sub>13</sub>(μ<sub>4</sub>-C<sub>7</sub>H<sub>7</sub>)<sub>6</sub>]<sup>2+</sup> (C<sub>7</sub>H<sub>7</sub> = tropylium) with an fcc-close-packed cuboctahedral Pd<sub>13</sub> core and isomers: theoretical insight into ligand-control of the Pd<sub>13</sub> core structure

Bo Zhu, Tetsuro Murahashi\* and Shigeyoshi Sakaki\*

25681



### Hematite photoanodes for water splitting from directed assembly of Prussian blue onto CuO–Sb<sub>2</sub>O<sub>5</sub>–SnO<sub>2</sub> ceramics

Alexander N. Bondarchuk\* and Frank Marken

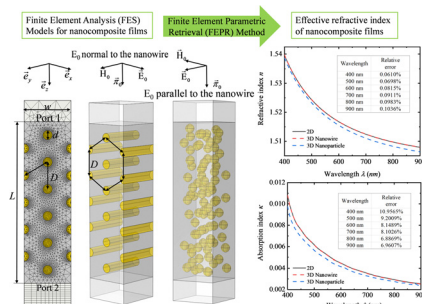




25689

## A novel theoretical method to determine the effective optical properties of high refractive index nanocomposites

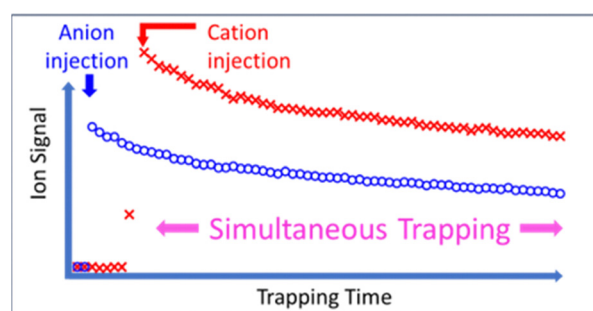
Xiaoning Li, Chengwei Jia, Chengchao Wang,\* Lanxin Ma and Linhua Liu\*



25701

## Simultaneous electrostatic trapping of merged cation & anion beams

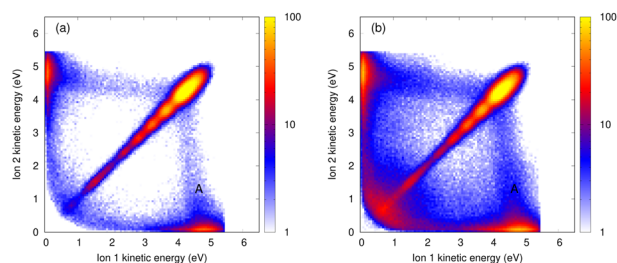
Alon Bogot, Oleg Lioubashevski, Oded Heber, Daniel Zajfman and Daniel Strasser\*



25711

## Interatomic Coulombic decay in small helium clusters

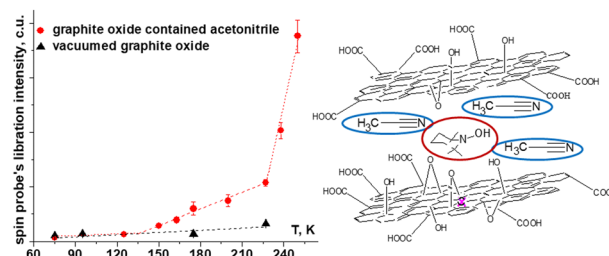
Sévan Kazandjian, Max Kircher, Gregor Kastirke, Joshua B. Williams, Markus Schöffler, Maksim Kunitski, Reinhard Dörner, Tsveta Miteva, Selma Engin, Florian Trinter,\* Till Jahnke\* and Nicolas Sisourat\*



25720

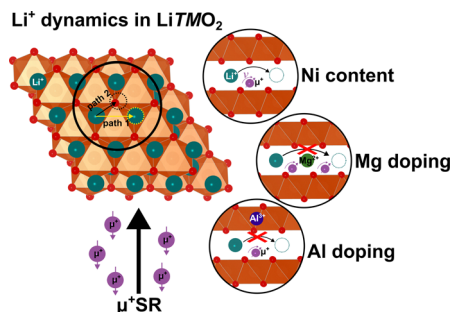
## Glass-like behavior of intercalated organic solvents in graphite oxide detected by spin-probe EPR

Victoria N. Syryamina,\* Dmitry A. Astvatsaturov, Sergei A. Dzuba and Natalia A. Chumakova



## RESEARCH PAPERS

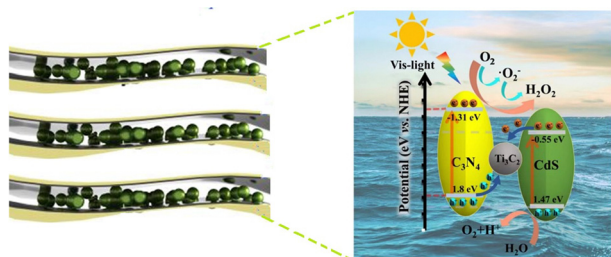
25728



### Elucidating local diffusion dynamics in nickel-rich layered oxide cathodes

Beth I. J. Johnston,\* Innes McClelland, Peter J. Baker and Serena A. Cussen\*

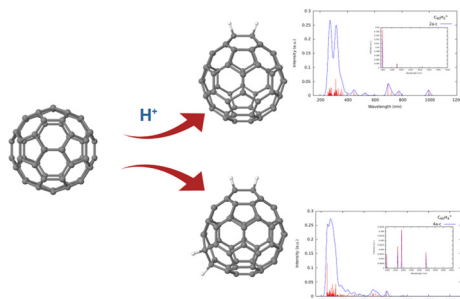
25734



### In situ fabrication of Z-scheme C<sub>3</sub>N<sub>4</sub>/Ti<sub>3</sub>C<sub>2</sub>/CdS for efficient photocatalytic hydrogen peroxide production

Jianrui Cao, Suyu Zhou, Junhao Cai, Junhe Han, Junhui Liu,\* Ruoping Li and Mingju Huang\*

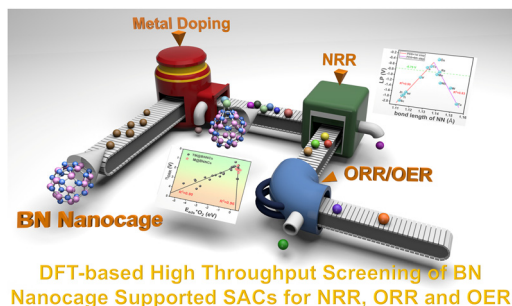
25746



### Gas-phase C<sub>60</sub>H<sub>n</sub><sup>+q</sup> ( $n = 0-4$ , $q = 0,1$ ) fullerenes and fulleranes: spectroscopic simulations shed light on cosmic molecular structures

Ricardo R. Oliveira,\* Germán Molpeceres,\* Ricardo Montserrat, Felipe Fantuzzi, Alexandre B. Rocha and Johannes Kästner

25761



### d- and p-Block single-atom catalysts supported by BN nanocages toward electrochemical reactions of N<sub>2</sub> and O<sub>2</sub>

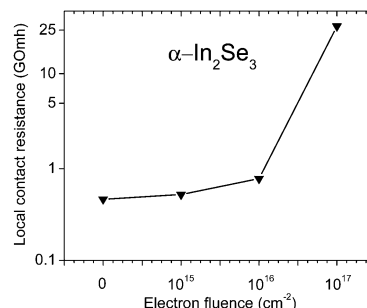
Chenhui Wang, Fan Huang, Haikuan Liang, Wei Nong, Fei Tian,\* Yan Li\* and Chengxin Wang



25772

### Effect of 10 MeV electron irradiation on the electrical properties of bulk $\alpha$ - $\text{In}_2\text{Se}_3$ crystals

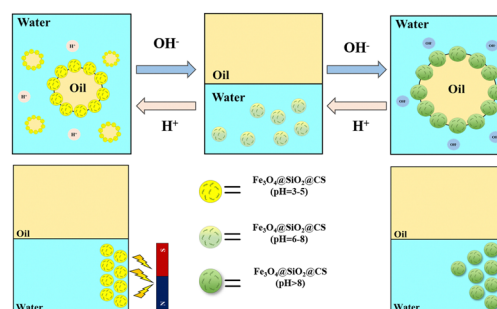
Alexey D. Lobanov,\* Yulia V. Korkh, Evgeny I. Patrakov, Vasily S. Gaviko, Maxim N. Sarychev, Vladimir Yu. Ivanov and Tatyana V. Kuznetsova



25780

### pH/magnetic dual responsive Pickering emulsion stabilized by $\text{Fe}_3\text{O}_4@ \text{SiO}_2@ \text{chitosan}$ nanoparticles

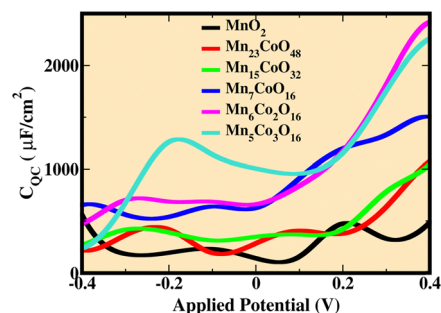
Runna He, Shuangqing Sun,\* Jianpeng Cui, Mingshuo Chi, Zhikun Wang and Songqing Hu



25789

### Theoretical investigation of quantum capacitance of Co-doped $\alpha$ - $\text{MnO}_2$ for supercapacitor applications using density functional theory

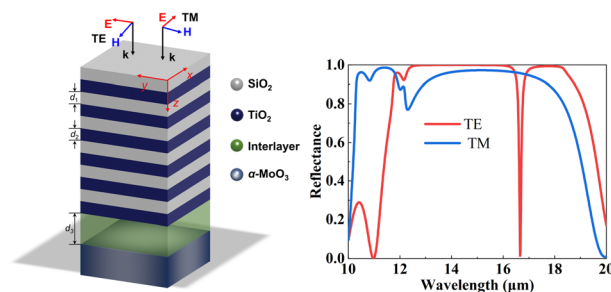
Ariya K. Vijayan, Sreehari M. S, Simran Kour, Saptarshi Ghosh Dastider, Krishnakanta Mondal and A. L. Sharma\*



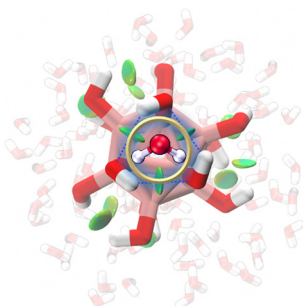
25803

### A polarization-dependent perfect absorber with high Q-factors enabled by Tamm phonon polaritons in hyperbolic materials

Didi Song, Biyuan Wu, Yufang Liu, Xiaohu Wu\* and Kun Yu\*



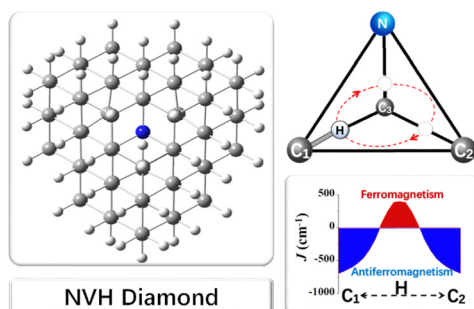
25810



### Locking water molecules *via* ternary O–H...O intramolecular hydrogen bonds in perhydroxylated *closo*-dodecaborate

Yanrong Jiang, Zhubin Hu, Cheng Zhong, Yan Yang, Xue-Bin Wang, Zhenrong Sun, Haitao Sun,\* Zhi Liu\* and Peng Peng\*

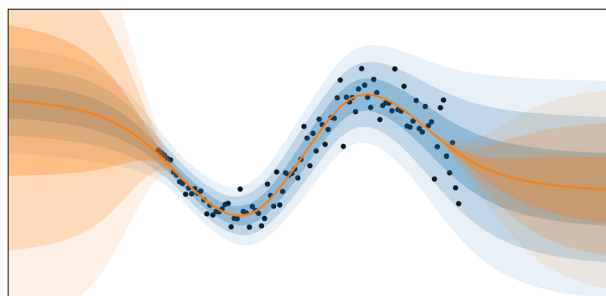
25818



### Hydrogen-migration governed dynamic magnetic coupling characteristics in nitrogen-vacancy-hydrogen nanodiamonds

Yamin Song, Xuexing Lin, Shaofen Yu, Yuxiang Bu and Xinyu Song\*

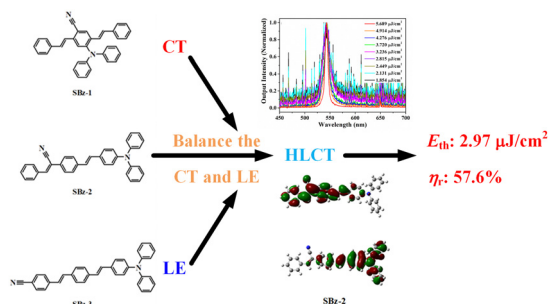
25828



### Graph neural network interatomic potential ensembles with calibrated aleatoric and epistemic uncertainty on energy and forces

Jonas Busk,\* Mikkel N. Schmidt, Ole Winther, Tejs Vegge and Peter Bjørn Jørgensen

25838



### Tailoring D–π–A architectures with hybridized local and charge transfer fluorophores exhibiting high electroluminescence exciton utilization and low threshold amplified spontaneous emission

Lin Ma, Yue Yu,\* Daokun Zhong, Chunrong Zhu, Xiaolong Yang, Zhao Feng, Guijiang Zhou\* and Zhaoxin Wu\*

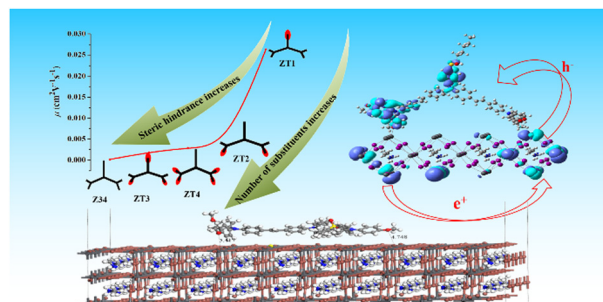


## RESEARCH PAPERS

25850

### Effect of steric hindrance and number of substituents on the transfer and interface properties of Y-shaped hole-transporting materials for perovskite solar cells

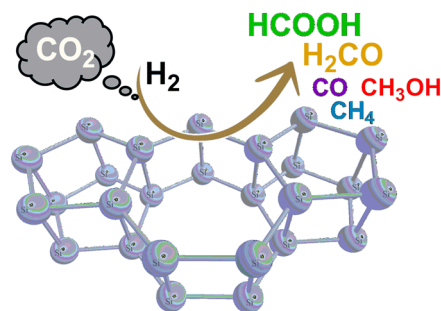
Zemin Zhang,\* Zetian Tang, Keliang Wang,\* Ping Wang and Jianfa Yang



25862

### Enhancing CO<sub>2</sub> reduction through the catalytic effect of a novel silicon haeckelite-inspired 2D material

Wilmer Esteban Vallejo Narváez,\* Cesar Gabriel Vera de la Garza and Serguei Fomine\*



25871

### Investigating the influence of substituent groups in TTM based radicals for the excitation process: a theoretical study

Lu-ran Fei, Jian Wang, Fu-quan Bai, Shi-ping Wang, Bin Hu, Chui-peng Kong\* and Hong-xing Zhang\*

