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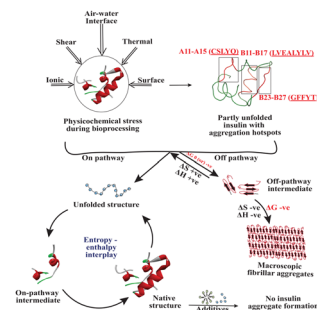
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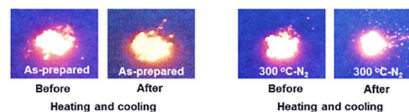
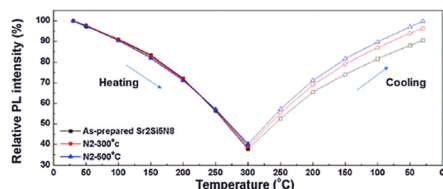
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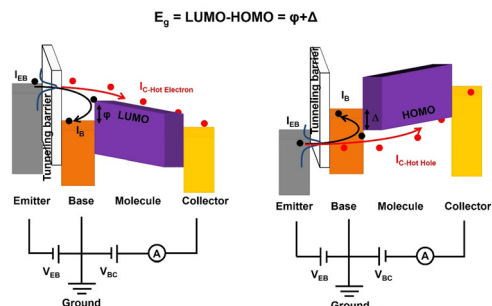
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## Going ballistic: a novel characterization for the electronic energy gap

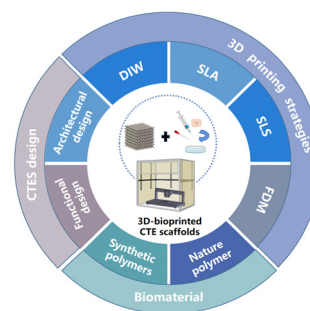
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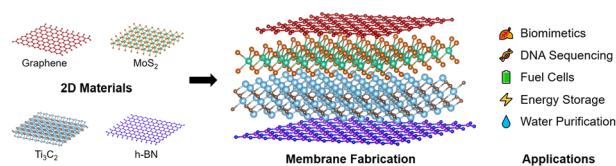
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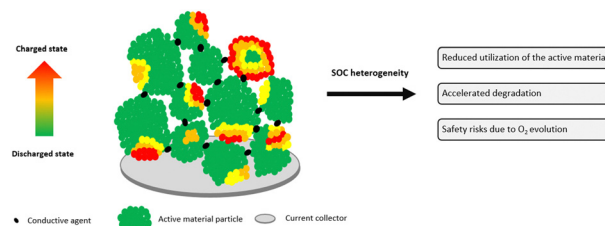
Selene Acosta, H. Joazet Ojeda-Galván and Mildred Quintana\*



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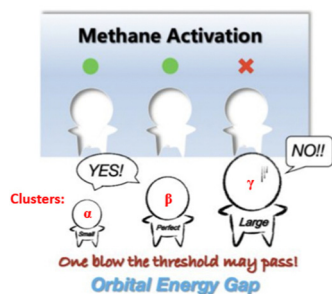
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Marc Vahnstiege, Martin Winter, Sascha Nowak\* and Simon Wiemers-Meyer



## COMMUNICATIONS

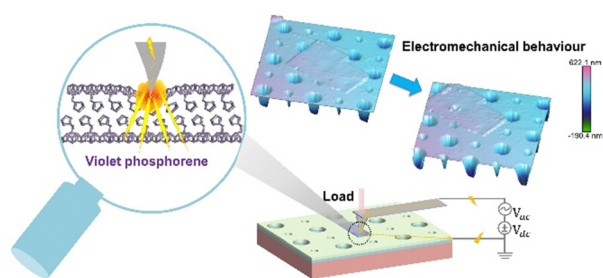
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### On the performance of the M–C (M = Fe, Ru, Os) unit toward methane activation

Shihan Li, Chao Qian, Xiao-Nan Wu\* and Shaodong Zhou\*

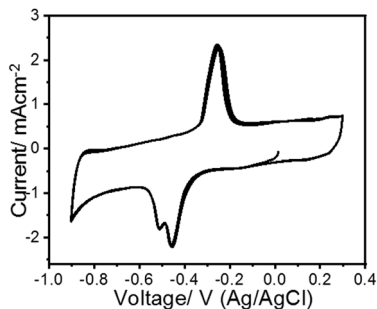
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### Electromechanical behaviour of violet phosphorene nanoflakes

Bo Zhang,\* Zhenyu Wang,\* Chengxiang Chen, Mengyue Gu, Jun Zhou and Jinying Zhang\*

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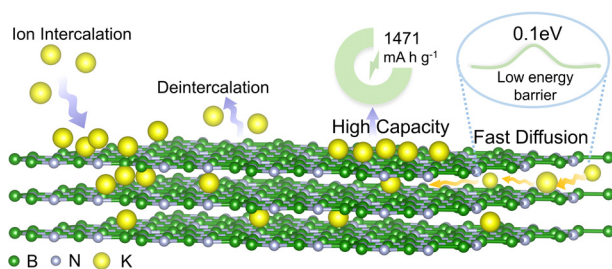


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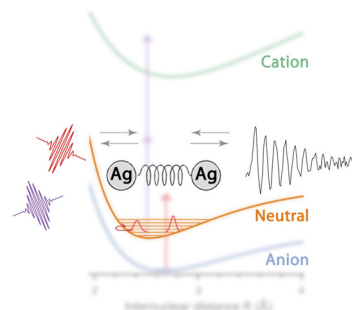


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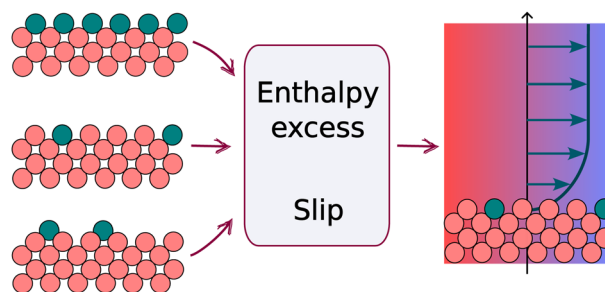
Jiaye Jin,\* Max Grellmann and Knut R. Asmis\*



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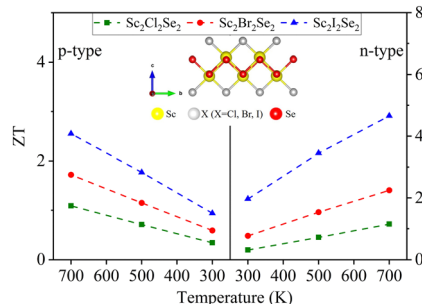
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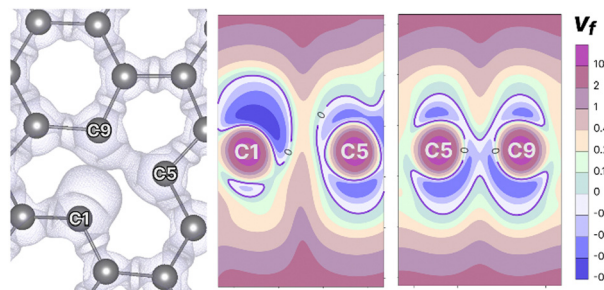
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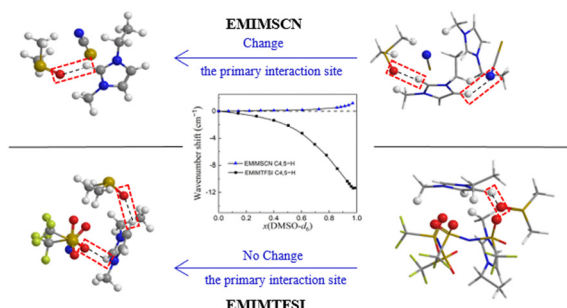
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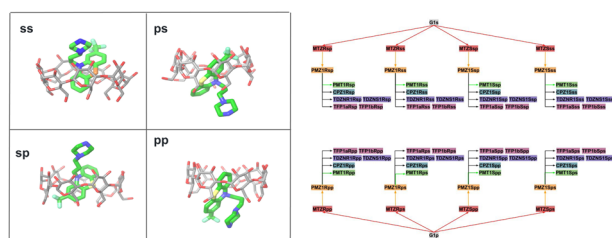
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Rui Zhao, Xianzhen Xu, Zonghua Wang, Yanzhen Zheng\* and Yu Zhou\*

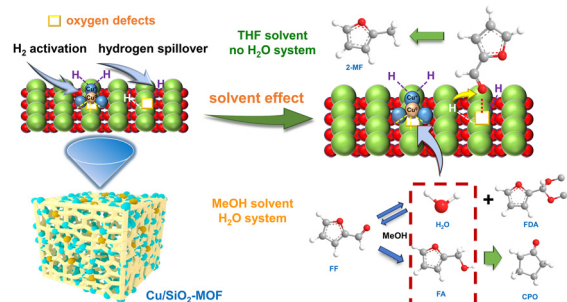
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Sheenam Khuttan, Solmaz Azimi, Joe Z. Wu, Sebastian Dick, Chuanjie Wu, Huafeng Xu and Emilio Gallicchio\*

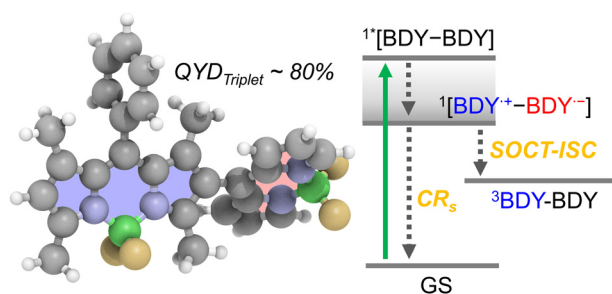
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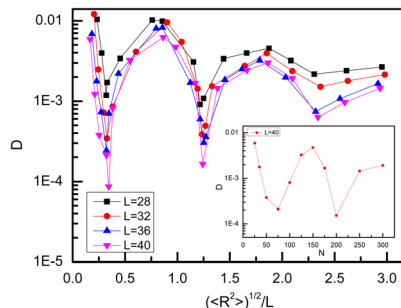
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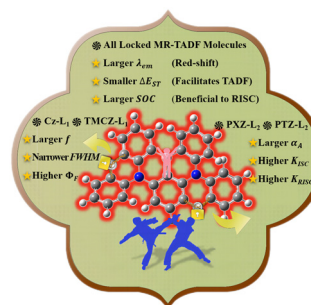
Jiaxin Wu, Zhiyong Yang, Xiaoou Cai and Linxi Zhang\*



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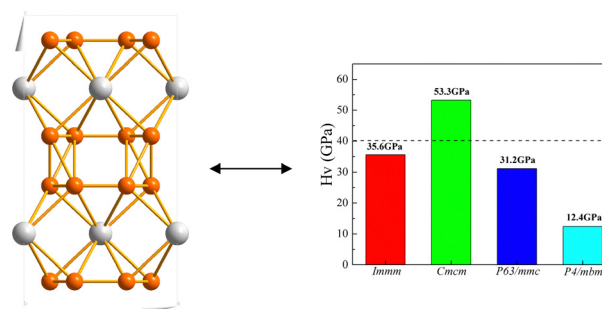
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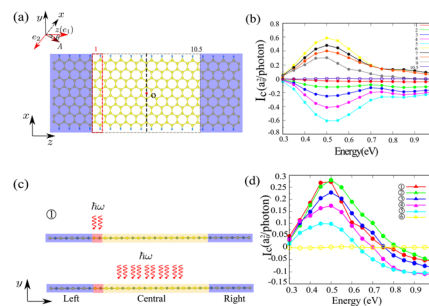
Yong Pan



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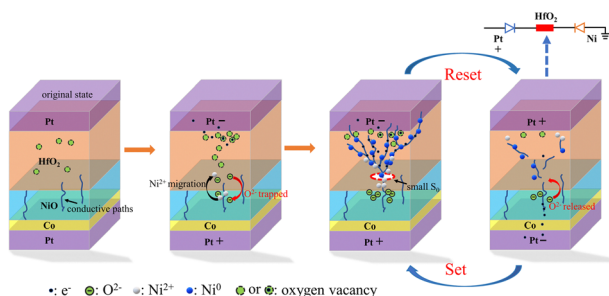
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Yuejun Li, Xiaofei Shang, Yan-Hong Zhou\* and Xiaohong Zheng\*



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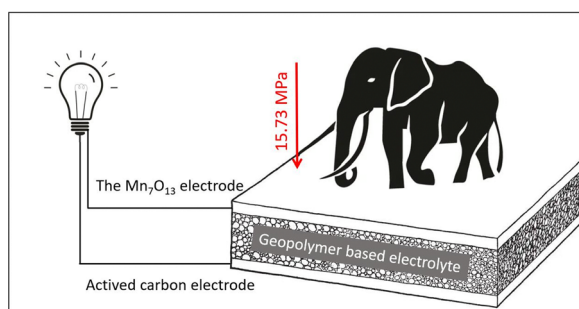
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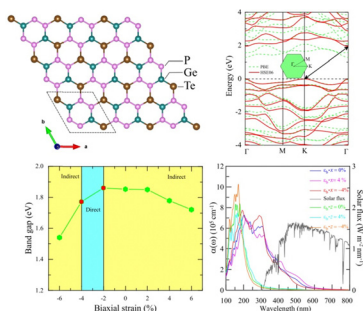
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Jing-Lei Yang, Wei-Bin Zhang,\* Shan-Shan Chai, Myat Myintzu Theint, Yi Yin, Ze-Qin Yang, Jia-Jun Li, Yu-Hui Yi and Xue-Jing Ma\*

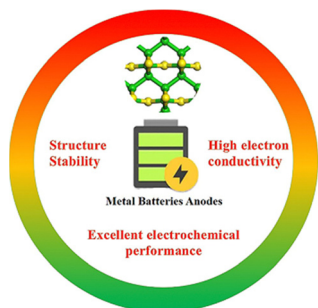
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Trung D. Pham\* and Tong D. Hien\*

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Danhong Wang, Zhifang Yang, Wenliang Li\* and Jingping Zhang\*

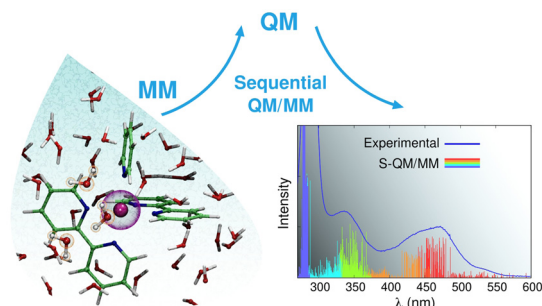


## RESEARCH PAPERS

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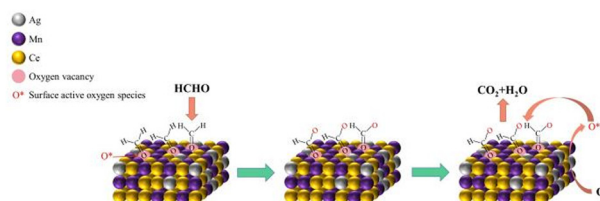
Leandro Rezende Franco,\* Kalil Cristhian Figueiredo Toledo, Tiago Araujo Matias, C. Moyses Araujo, Koiti Araki and Kaline Coutinho



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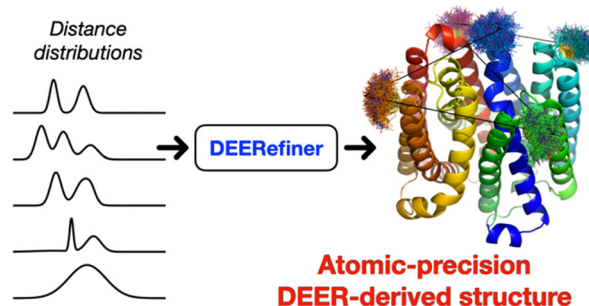
Chaomin Duan, Yanlin Zhou, Mianwu Meng,\* Huang Huang,\* Hua Ding, Qi Zhang, Renyuan Huang and Mengjuan Yan



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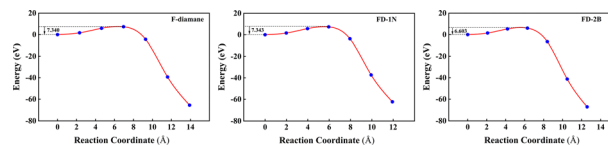
Te-Yu Kao and Yun-Wei Chiang\*



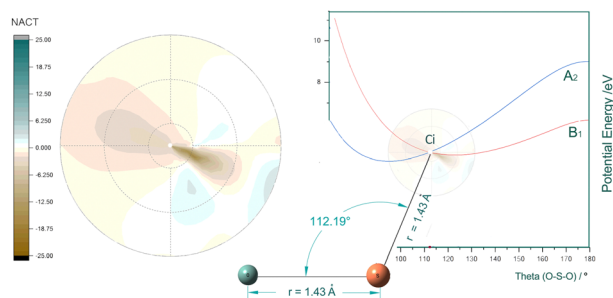
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### Structural stability and electronic and mechanical properties of nitrogen- and boron-doped fluorinated diamane

Lilin Gao, Yanning Liu, Yaqi Liang, Nan Gao,\* Junsong Liu\* and Hongdong Li\*



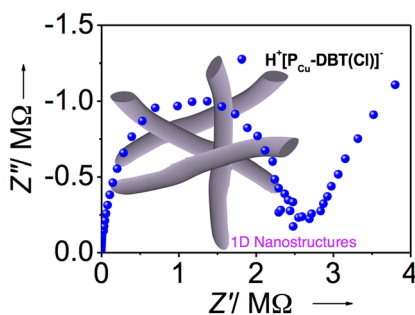
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### Non-adiabatic coupling in the potential energy surfaces of $\text{SO}_2$ molecule

Sedigheh Pourestarabadi and Maryam Dehestani\*

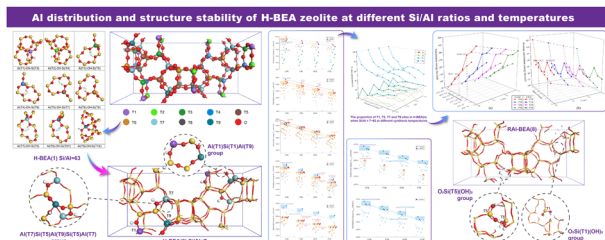
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### Conducting 1D nanostructures from light-stimulated copper-metallated porphyrin-dibenzothiophene

Yelukala Ramakrishna, Madarapu Naresh, Botta Bhavani and Seelam Prasanthkumar\*

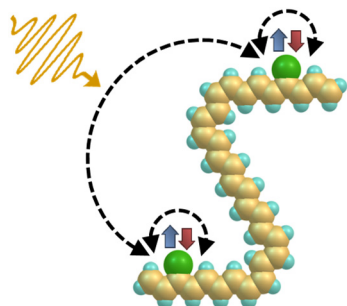
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### Al distribution and structural stability of H-BEA zeolites at different Si/Al ratios and temperatures: a first-principles study

Changdong Li, Xiuqin Dong, Haipeng Yu and Yingzhe Yu\*

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### Laser-induced ultrafast spin-transfer processes in non-linear zigzag carbon chain systems

Mohamed Barhoumi, Jing Liu, Georgios Lefkidis\* and Wolfgang Hübner

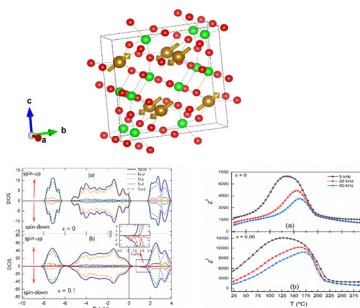


## RESEARCH PAPERS

24581

**Experimental and computational study on the influence of cobalt substitution on the structural, impedance, electronic, magnetic, and optical properties of pseudobrookite-structured  $\text{Fe}_2\text{TiO}_5$** 

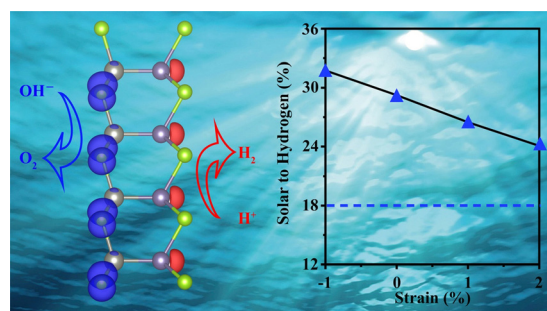
M. Naveed-Ul-Haq,\* Anum Shafiq, Layiq Zia and Arif Mumtaz



24594

 **$\text{ZnGeSe}_2$  monolayer: water-splitting photocatalyst with ultrahigh solar conversion efficiency**

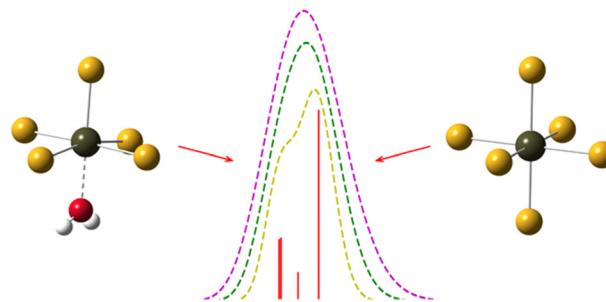
Guoting Nan, Wei Zhang, Xiaojun Yan, Xi Qin, Song Wu, Rufe Tang, Ming-Xia Tang, Lei Hu,\* Lili Liu, Shifa Wang, Yuming Feng\* and Wencai Yi\*



24603

**Excited states of polonium(IV): electron correlation and spin-orbit coupling in the  $\text{Po}^{4+}$  free ion and in the bare and solvated  $[\text{PoCl}_5]^-$  and  $[\text{PoCl}_6]^{2-}$  complexes**

Nadiya Zhutova, Florent Réal, Eric Renault, Valérie Vallet\* and Rémi Maurice\*



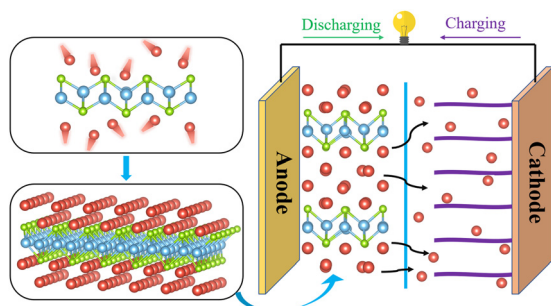
24613

**Waste dry cell derived photo-reduced graphene oxide and polyoxometalate composite for solid-state supercapacitor applications**

Sukanya Maity, Bhimaraya R Biradar, Saurabh Srivastava, Pranay R. Chandewar, Debaprasad Shee, Partha Pratim Das\* and Sib Sankar Mal\*



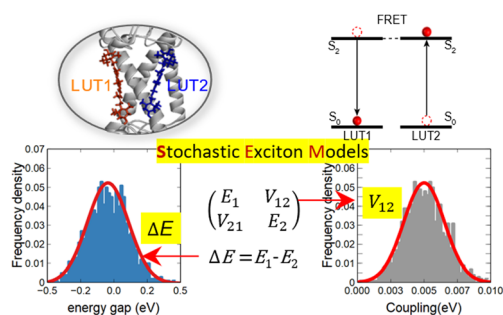
24625



### A TiSe monolayer as a superior anode for applications of Li/Na/K-ion batteries

Mengke Wang, Shan Wang, Yunye Liang, Yiqun Xie, Xiang Ye\* and Shoutian Sun\*

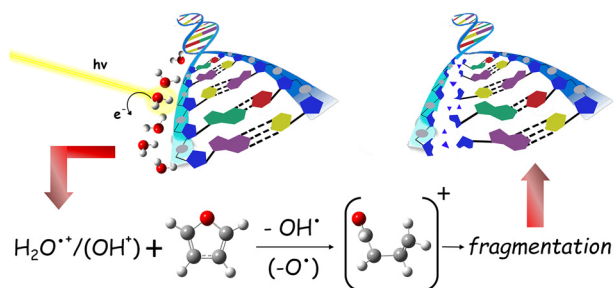
24636



### Intermolecular resonance energy transfer between two lutein pigments in light-harvesting complex II studied by frenkel exciton models

Jiarui Li, Tao Zeng, Yu Zhai, Zexing Qu\* and Hui Li\*

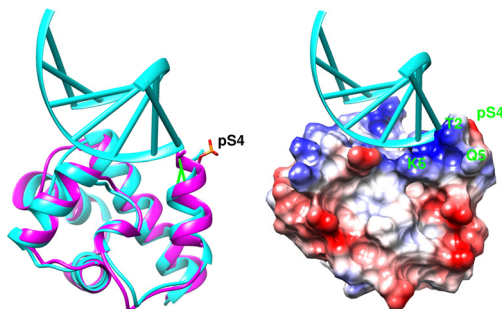
24643



### H<sub>2</sub>O<sup>+</sup> and OH<sup>+</sup> reactivity *versus* furan: experimental low energy absolute cross sections for modeling radiation damage

Daniela Ascenzi, Ewa Erdmann, Paola Bolognesi, Lorenzo Avaldi, Mattea Carmen Castrovilli, Roland Thissen, Claire Romanzin, Christian Alcaraz, Ismanuel Rabadan, Luis Mendez, Sergio Diaz-Tendero\* and Antonella Cartoni\*

24657



### Mono-phosphorylation at Ser4 of barrier-to-autointegration factor (Banf1) significantly reduces its DNA binding capability by inducing critical changes in its local conformation and DNA binding surface

Ming Tang,\* Amila Suraweera, Xuqiang Nie, Zilin Li, Pinglin Lai, James W. Wells, Kenneth J. O'Byrne, Robert J Woods, Emma Bolderson\* and Derek J Richard\*

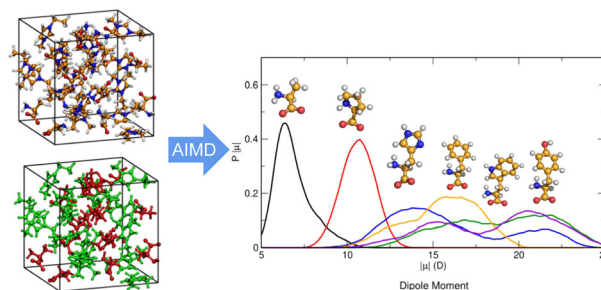


## RESEARCH PAPERS

24678

## Locality in amino-acid based imidazolium ionic liquids

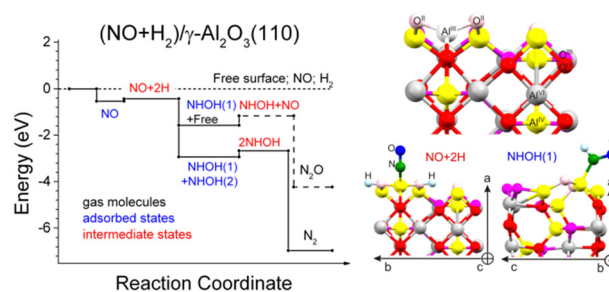
Wenbo Dong, Vahideh Alizadeh, Jan Blasius, Luke Wylie, Leonard Dick, Zhijie Fan and Barbara Kirchner\*



24686

Catalytic activity of  $\gamma$ - $\text{Al}_2\text{O}_3(110)$  in the  $\text{NO} + \text{H}_2$  reaction: a DFT study

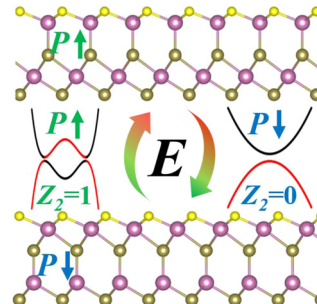
Alexander Cholach



24696

Non-volatile control of topological phase transition in an asymmetric ferroelectric  $\text{In}_2\text{Te}_2\text{S}$  monolayer

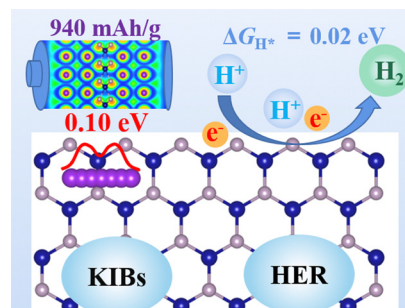
Guang Song,\* Yangyang Wu, Lei Cao, Guannan Li, Bingwen Zhang, Feng Liang and Benling Gao



24705

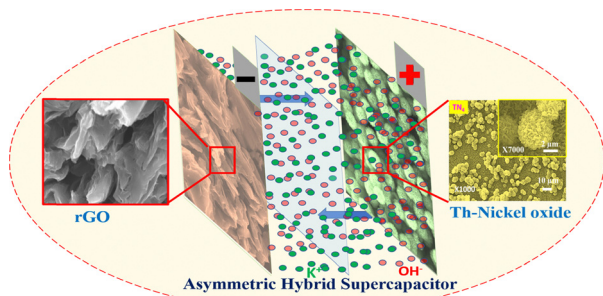
Metallic  $\text{CrP}_2$  monolayer: potential applications in energy storage and conversion

Jiayu Gao, Wenyan Zhang, Xu Yan, Xiaohua Zhang, Sheng Wang and Guochun Yang\*



## RESEARCH PAPERS

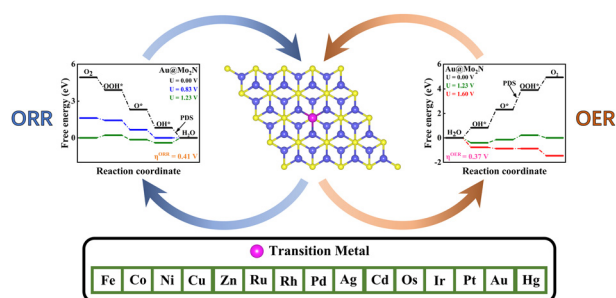
24712



### Porous 3D columnar-sphere of NiO nanomaterials synthesized for supercapacitors via hydrothermal route: impact of thiourea concentration

Amar L. Jadhav, Sharad L. Jadhav, Bhalchandra K. Mandlekar and Anamika V. Kadam\*

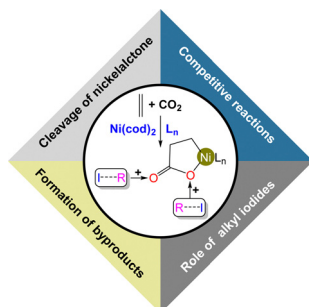
24721



### Theoretical study of Mo<sub>2</sub>N supported transition metal single-atom catalyst for OER/ORR bifunctional electrocatalysis

Long Lin, Xiaoqin Long, Xinyu Yang, Pei Shi and Linlin Su\*

24733

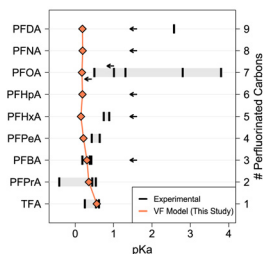
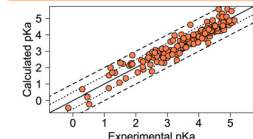
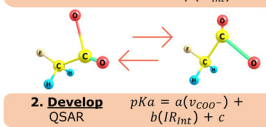


### Mechanistic study on the formation of the alkyl acrylates from CO<sub>2</sub>, ethylene and alkyl iodides over nickel-based catalyst

Youcai Zhu, Yue Mu, Li Sun, Zuoxiang Zeng and Zhen Liu\*

24745

- 1. Calculate** Vibrational Frequency ( $\nu_{COO^-}$ ) and Infrared Intensity ( $I_{R_{int}}$ )
- 2. Develop** QSAR  $pK_a = a(\nu_{COO^-}) + b(I_{R_{int}}) + c$
- 3. Apply** QSAR to perfluorinated carboxylic acids (PFCA) and other PFAS



### $pK_a$ prediction of per- and polyfluoroalkyl acids in water using *in silico* gas phase stretching vibrational frequencies and infrared intensities

Jimmy Murillo-Gelvez, Olga Dmitrenko, Tiffany L. Torralba-Sanchez, Paul G. Tratnyek and Dominic M. Di Toro\*

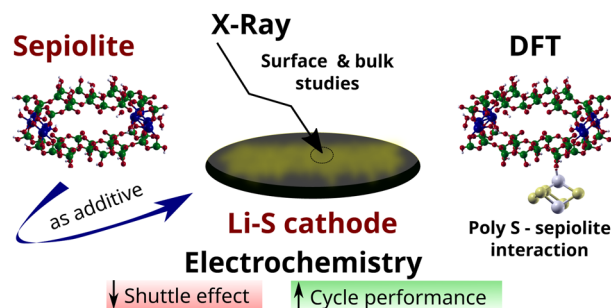


## RESEARCH PAPERS

24761

### Sepiolite as a novel polysulfide trapper for energy applications: an electrochemical, X-ray spectroscopic and DFT study

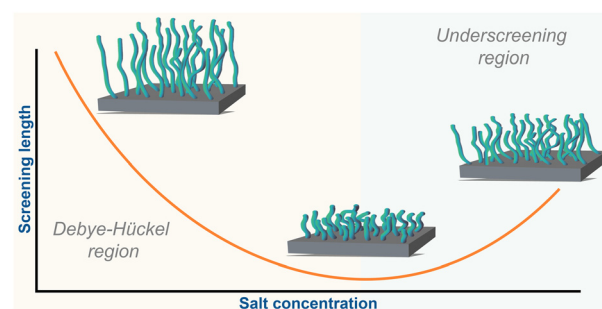
Francisco Javier García-Soriano,\* Sergio Andrés Ceppi, Fernando Pablo Cometto, Emiliano Nicolás Primo, Daniel Eugenio Barraco, Ezequiel Pedro Marcos Leiva, Guillermina Leticia Luque, Guillermo Stutz, German Lener\* and María Victoria Bracamonte\*



24770

### Underscreening in concentrated electrolytes: re-entrant swelling in polyelectrolyte brushes

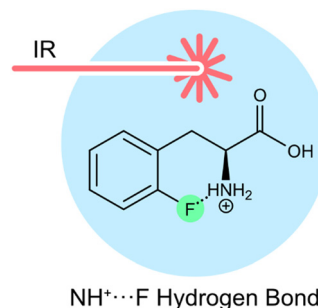
Hayden Robertson, Gareth R. Elliott, Andrew R. J. Nelson, Anton P. Le Brun, Grant B. Webber, Stuart W. Prescott, Vincent S. J. Craig, Erica J. Wanless and Joshua D. Willott\*



24783

### Cryogenic infrared spectroscopy reveals remarkably short $\text{NH}^+ \cdots \text{F}$ hydrogen bonds in fluorinated phenylalanines

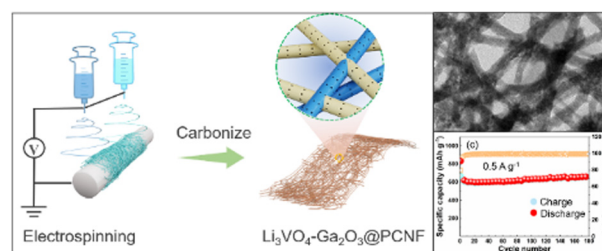
Marc Safferthal, Kim Greis, Rayoon Chang, Carla Kirschbaum, Waldemar Hoffmann, Gerard Meijer, Gert von Helden and Kevin Pagel\*



24789

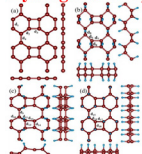
### Heterostructured $\text{Li}_3\text{VO}_4\text{-Ga}_2\text{O}_3$ -embedded porous carbon nanofibers as advanced anode materials for lithium-ion batteries

Canyang Chen, Cunyuan Pei,\* Song Yang, Huijuan Ma, Dongmei Zhang, Bing Sun and Shibing Ni\*



24797

## Hydrogenated biphenylene



$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

DFT (VASP)

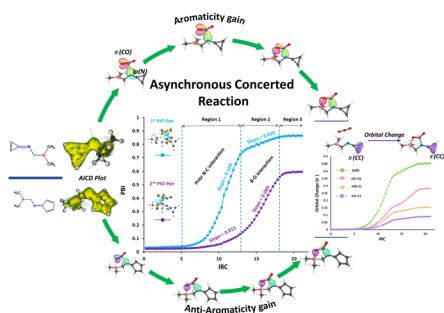


High Stability  
 Negative Poisson's ratio  
 Anisotropy  
 Direct band gap

### Structural, mechanical, electronic and optical properties of biphenylene hydrogenation: a first-principles study

Kai Chen, Jian Zhou, Wuyan Zhao, Riyi Yang, Chong Qiao, Wan-Sheng Su,\* Yuxiang Zheng, Rongjun Zhang, Liangyao Chen and Songyou Wang\*

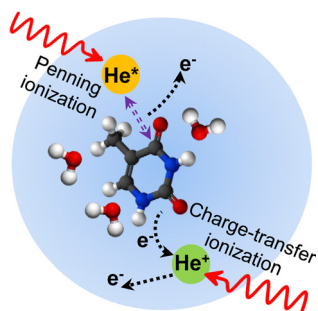
24809



### PIO and IBO analysis to unravel the hidden details of the CO<sub>2</sub> sequestration mechanism of aromatically tempered N/B-based IFLPs

Mohammad Faizan, Adarsh Kumar, Mucherla Raghasudha and Ravinder Pawar\*

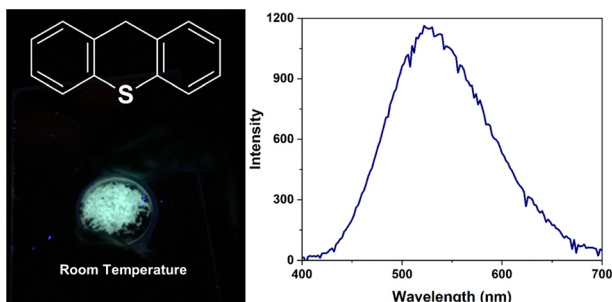
24819



### Secondary ionization of pyrimidine nucleobases and their microhydrated derivatives in helium nanodroplets

Jakob D. Asmussen, Abdul R. Abid, Akgash Sundaralingam, Björn Bastian, Keshav Sishodia, Subhendu De, Ltaief Ben Ltaief, Sivarama Krishnan, Henrik B. Pedersen and Marcel Mudrich\*

24829



### Photophysical investigation into room-temperature emission from xanthene derivatives

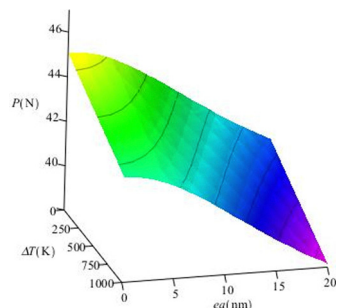
Kristen Harrington, David T. Hogan, Todd C. Sutherland\* and Kevin Stamplecoskie\*



24838

### A nonlocal strain gradient shell model with the surface effect for buckling analysis of a magneto-electro-thermo-elastic cylindrical nanoshell subjected to axial load

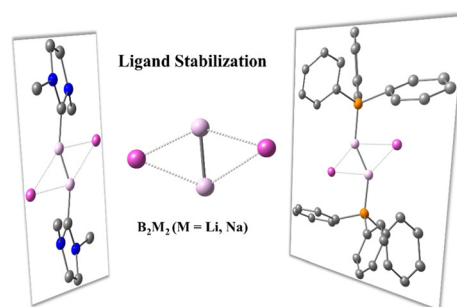
Yifei Gui and Zhisong Li\*



24853

### Mimicking the C<sub>2</sub> molecule: M<sub>2</sub>B<sub>2</sub> and M<sub>3</sub>B<sub>2</sub><sup>+</sup> clusters (M = Li, Na) and the reactivity of the N-heterocyclic carbene bound Li<sub>2</sub>B<sub>2</sub> complex

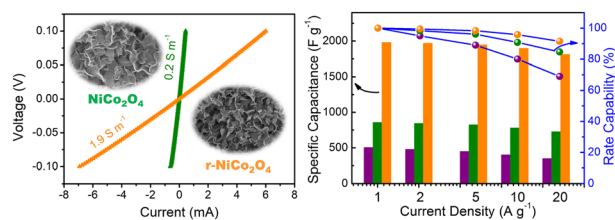
Yu-qian Liu, Gai-ru Yan, Li-juan Cui, Bing Yan, Sudip Pan\* and Zhong-hua Cui\*



24862

### Oxygen defect-mediated NiCo<sub>2</sub>O<sub>4</sub> nanosheets as the electrode for pseudocapacitors with improved rate capability

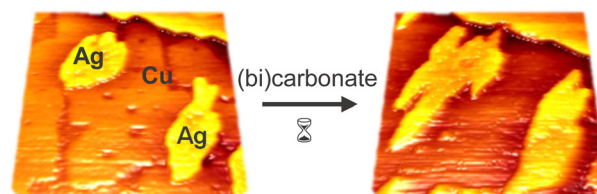
Wen You, Mengyuan Li, Qiong Li, Jizhou Jiang, Kun Xiang\* and Mingjiang Xie\*



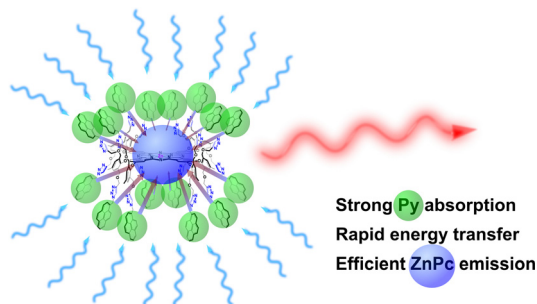
24871

### In situ scanning tunneling microscopy studies of carbonate-induced restructuring of Ag-decorated Cu(100) electrodes

Reihaneh Amirbeigi-arab and Olaf M. Magnussen\*



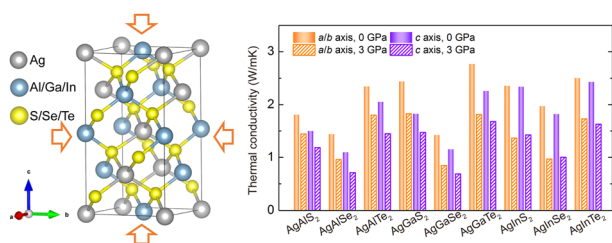
24878



### Covalently linked pyrene antennas for optically dense yet aggregation-resistant light-harvesting systems

Lubna Salah, Saad Makhseed, Basma Ghazal, Ahmed Abdel Nazeer, Marc K. Etherington, Carlito S. Ponseca Jr., Chunyong Li, Andrew P. Monkman, Andrew Danos\* and Ali Shuaib\*

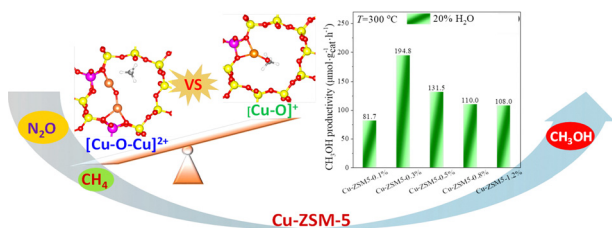
24883



### Soft phonon modes lead to suppressed thermal conductivity in Ag-based chalcopyrites under high pressure

Kunpeng Yuan, Xiaoliang Zhang,\* Yufei Gao and Dawei Tang\*

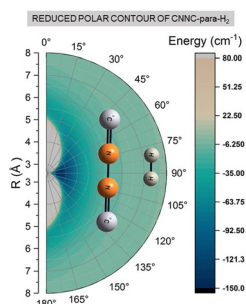
24894



### Mechanistic insight into the effect of active site motif structures on direct oxidation of methane to methanol over Cu-ZSM-5

Chengna Dai, Yuchan Zhang, Ning Liu,\* Gangqiang Yu, Ning Wang, Ruinian Xu and Biaohua Chen

24904



### New potential energy surface and rotational deexcitation cross-sections of CNNC by *para*-H<sub>2</sub> ( $j_p = 0$ )

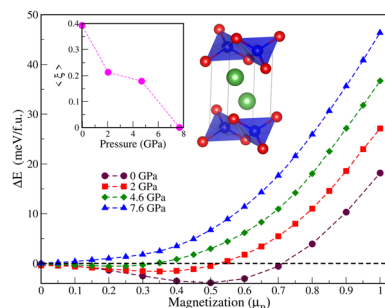
Ritika and T. J. Dhillip Kumar\*



24912

## Proximity of superconducting LaCoSi to a ferromagnetic quantum critical point

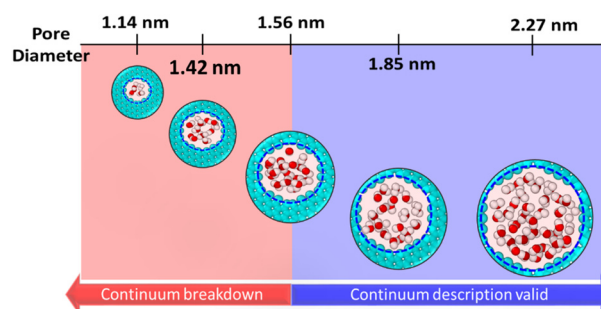
Himanshu and J. J. Pulikkotil\*



24919

## The validity of the continuum modeling limit in a single pore flows to the molecular scale

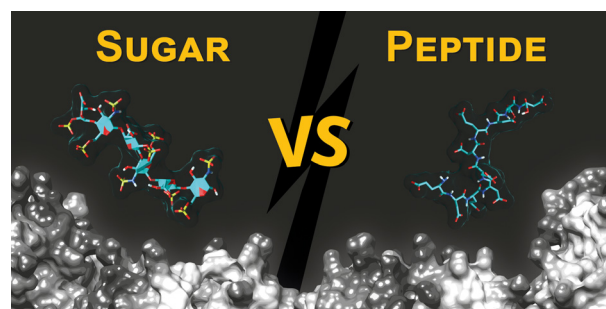
Jaber Al Hossain and BoHung Kim\*



24930

## Ligand binding of interleukin-8: a comparison of glycosaminoglycans and acidic peptides

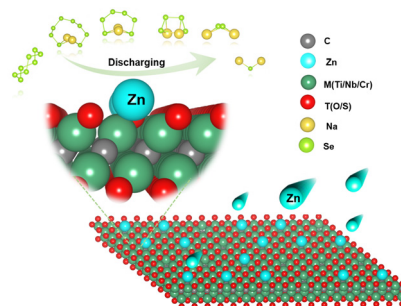
Christian Schulze, Annemarie Danielsson, Adam Liwo, Daniel Huster, Sergey A. Samsonov\* and Anja Penk\*



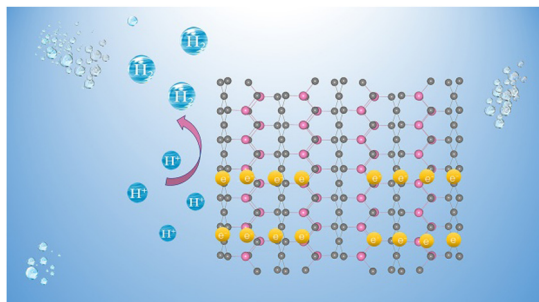
24948

## Rational design of MXene-based single atom catalysts for Na–Se batteries from sabatier principle

Chunlei Wei, MengMeng Ge, Timing Fang,\* Xiao Tang and Xiaomin Liu\*



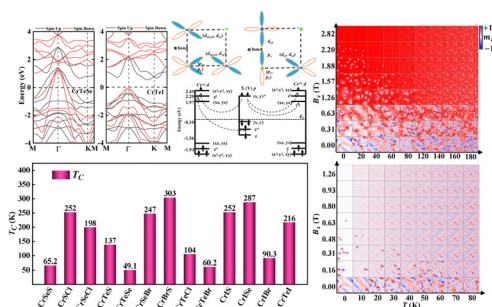
24960



### Photocatalytic water splitting for hydrogen production with high efficiency monolayer $\text{In}_2\text{Te}_5$ : a theoretical study

Cong Zhang, Meiping Tan, Xin Lu, Wenzhuo Li, Yang Yu, Qiang Wang, Wenjun Zhang, Xiaole Qiu and Hongchao Yang\*

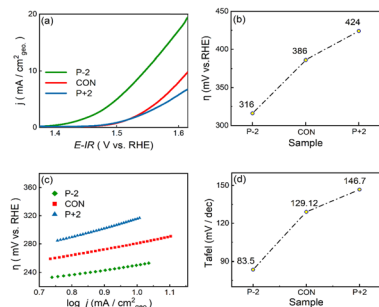
24968



### Electronic properties, skyrmions and bimerons in Janus $\text{CrXY}$ ( $X, Y = \text{S, Se, Te, Cl, Br, I}$ , and $X \neq Y$ ) monolayers

Zhihao Guan, Zhong Shen, Yufei Xue, Tingting Zhong, Xiaoping Wu and Changsheng Song\*

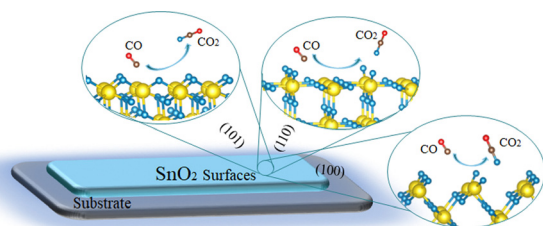
24976



### Modulating the oxygen evolution reaction activity of $\text{SrIrO}_3/\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.7}\text{Ti}_{0.3}\text{O}_3$ catalysts using electric-field polarization

Anxin Meng, Jiabao Ding, Caiqin Luo, Mian Qin\* and Weifeng Zhang\*

24985



### Preferred surface orientation for CO oxidation on $\text{SnO}_2$ surfaces

Zineb Kerrami,\* Anass Sibari, Mohammed Benaissa and Abdelkader Kara\*

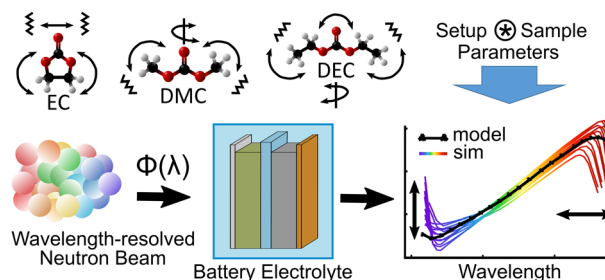


## RESEARCH PAPERS

24993

## Prospects of spectroscopic neutron imaging: optimizing experimental setups in battery electrolyte research

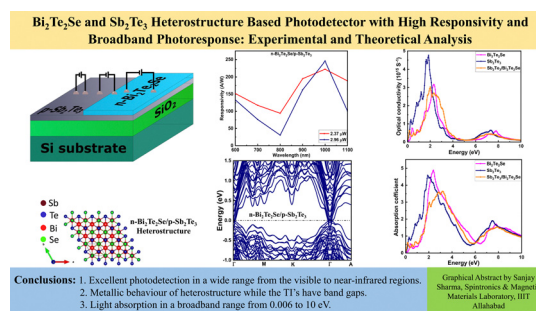
E. Ricardo Carreón Ruiz, Natalie Stalder, Jongmin Lee, Lorenz Gubler and Pierre Boillat\*



25008

Bi<sub>2</sub>Te<sub>2</sub>Se and Sb<sub>2</sub>Te<sub>3</sub> heterostructure based photodetectors with high responsivity and broadband photoresponse: experimental and theoretical analysis

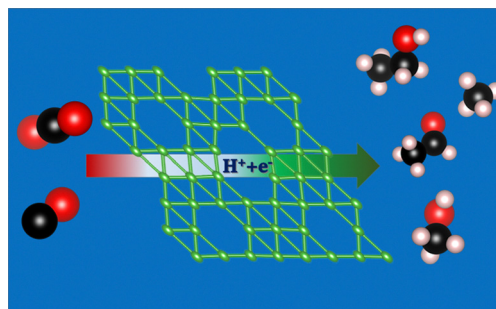
Sandeep Kumar Verma, Sanjay Sharma, Gyanendra Kumar Maurya, Vidushi Gautam, Roshani Singh, Ajeet Singh, Kavindra Kandpal, Pramod Kumar,\* Arun Kumar and Claudia Wiemer\*



25018

Single B-vacancy enriched  $\alpha_1$ -borophene sheet: an efficient metal-free electrocatalyst for CO<sub>2</sub> reduction

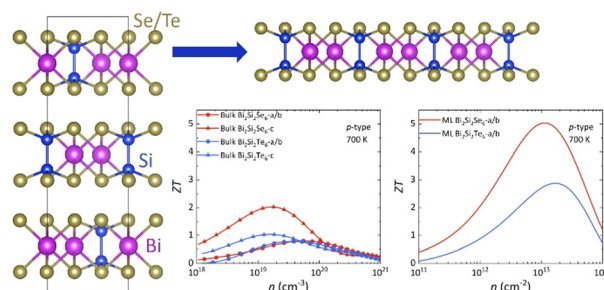
Prodyut Roy, Sourav Ghoshal, Anup Pramanik and Pranab Sarkar\*



25029

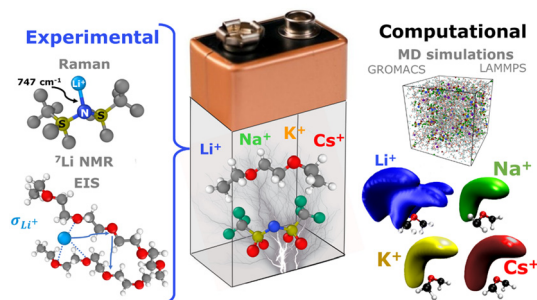
Dimensionality reduction induced synergetic optimization of the thermoelectric properties in Bi<sub>2</sub>Si<sub>2</sub>X<sub>6</sub> (X = Se, Te) monolayers

Tingting Zhang, Suiting Ning, Ziyi Zhang, Ning Qi and Zhiqian Chen\*



## RESEARCH PAPERS

25038



### Synergistic theoretical and experimental study on the ion dynamics of bis(trifluoromethanesulfonyl)-imide-based alkali metal salts for solid polymer electrolytes

Brigette Althea Fortuin, Jon Otegi,  
 Juan Miguel López del Amo,  
 Sergio Rodríguez Peña, Leire Meabe, Hegoi Manzano,\*  
 María Martínez-Ibañez\* and Javier Carrasco\*

## CORRECTION

25055

### Correction: Lone pair driven anisotropy in antimony chalcogenide semiconductors

Xinwei Wang, Zhenzhu Li, Seán R. Kavanagh, Alex M. Ganose and Aron Walsh\*

