

## IN THIS ISSUE

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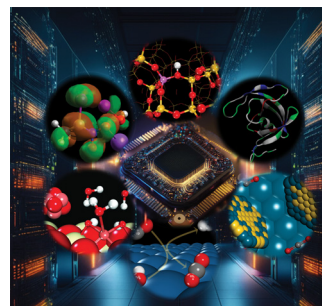
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*Phys. Chem. Chem. Phys.*,  
2023, 25, 20782.

## EDITORIAL

20775

### Computational modelling in catalytic science

C. Richard A. Catlow,\* Arunabhiram Chutia\* and  
Matthew G. Quesne\*

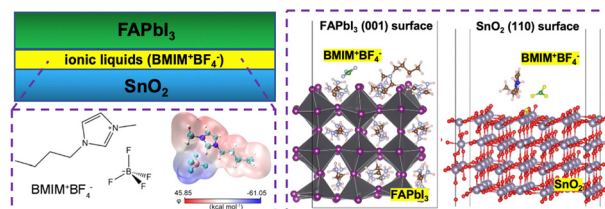


## COMMUNICATION

20777

### Unraveling the dynamic behaviors of BF<sub>4</sub>-based ionic liquids at the SnO<sub>2</sub>/FAPbI<sub>3</sub> interface using *ab initio* molecular dynamics simulations

Jinge Han, Hongbin Xiao,\* Yanru Guo, Xue Liu,  
Zhigang Zang and Ru Li\*



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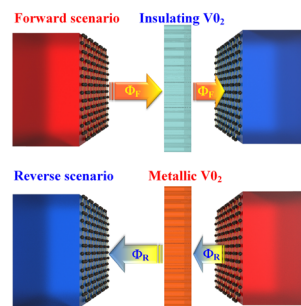


## RESEARCH PAPERS

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### Performance improvement of three-body radiative diodes driven by graphene surface plasmon polaritons

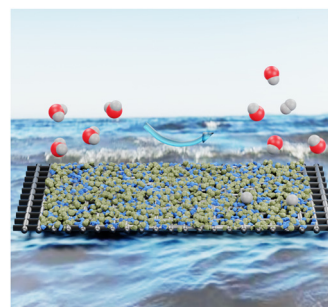
Ming-Jian He, Xue Guo, Hong Qi,\* Zhi-Heng Zheng,\*  
Mauro Antezza and He-Ping Tan



20794

### Scalable production of foam-like nickel–molybdenum coatings via plasma spraying as bifunctional electrocatalysts for water splitting

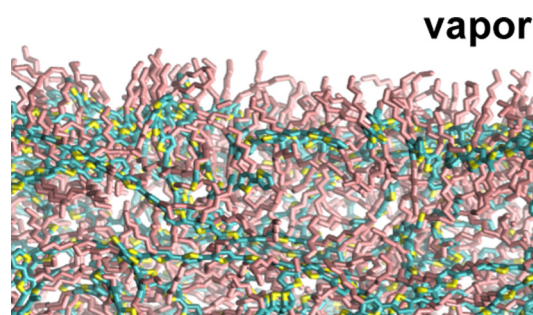
Xiuyu Wu, Alexis Piñeiro-García, Mouna Rafei,  
Nicolas Boulanger, Esdras Josué Canto-Aguilar and  
Eduardo Gracia-Espino\*



20808

### Accumulation and ordering of P3HT oligomers at the liquid–vapor interface with implications for thin-film morphology

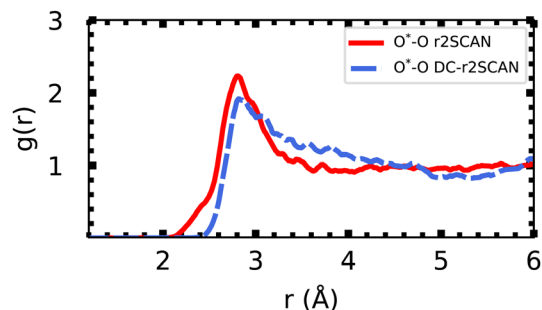
Jakub K. Sowa, Thomas C. Allen and Peter J. Rossky\*



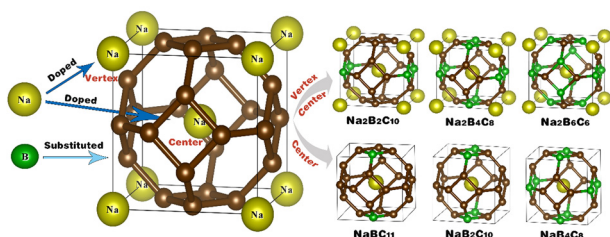
20817

### Radicals in aqueous solution: assessment of density-corrected SCAN functional

Fabian Belleflamme and Jürg Hutter\*



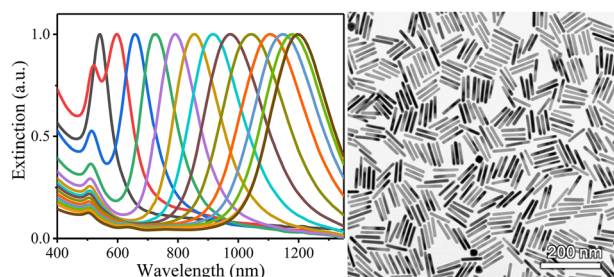
20837



### Prediction of potential hard sodium carbaboride compounds assuming sp<sup>3</sup>-bonded covalent clathrates

Ailing Liu, Xiaoran Cheng, Xingyu Wang, Yutong Zou and Miao Zhang\*

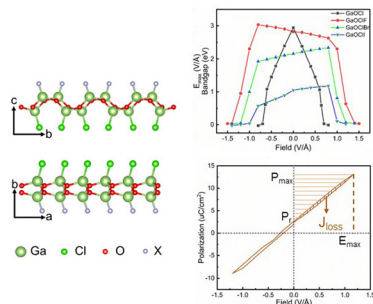
20843



### Controlled synthesis of monodisperse gold nanorods with a small diameter of around 10 nm and largest plasmon wavelength of 1200 nm

Anhua Wei, Jingfang OuYang, Yuyang Guo, Suju Jiang, Feifei Chen, Jun Huang, Qi Xiao and Zihua Wu\*

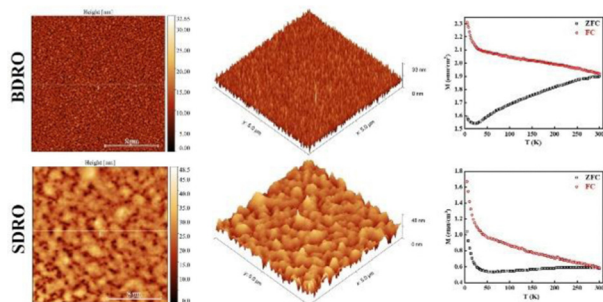
20854



### Janus GaOCIX (X = F, Br, and I) monolayers as predicted using first-principles calculations: a novel class of nanodielectrics with superior energy storage properties

Shujuan Jiang and Guangping Zheng\*

20863



### Integrated experimental and theoretical studies on structural and magnetic properties of thin films of double perovskite ruthenates: Ba<sub>2</sub>DyRuO<sub>6</sub> & Sr<sub>2</sub>DyRuO<sub>6</sub>

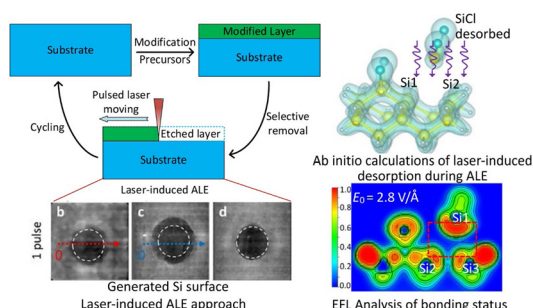
Sahil Dani, Rakesh Kumar, Hitesh Sharma, R J Choudhary, Navdeep Goyal, Pawanpreet Kaur and Rabia Pandit\*



20871

## Ab initio simulations of ultrashort laser pulse interaction with Cl–Si(100): implications for atomic layer etching

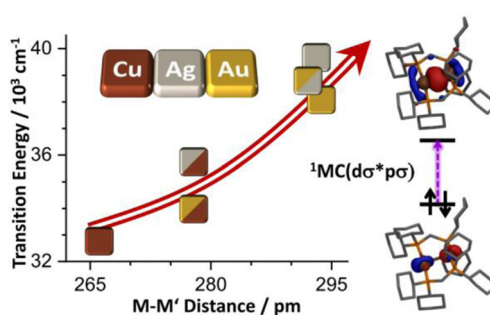
Peizhi Wang and Fengzhou Fang\*



20880

## Electronic spectroscopy of homo- and heterometallic binuclear coinage metal phosphine complexes in isolation

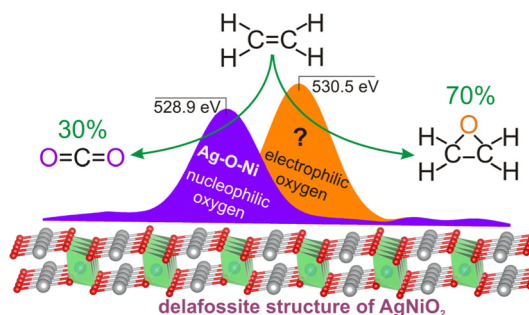
Marcel J. P. Schmitt, Sebastian V. Kruppa, Simon P. Walg, Werner R. Thiel, Wim Klopper\* and Christoph Riehn\*



20892

## Room temperature epoxidation of ethylene over delafossite-based AgNiO<sub>2</sub> nanoparticles

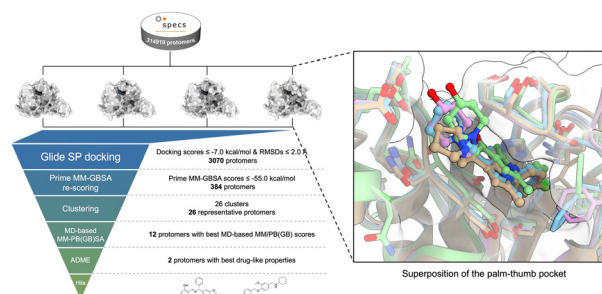
Dmitry A. Svintsitskiy,\* Mikhail K. Lazarev, Elena M. Slavinskaya, Elizaveta A. Fedorova, Tatyana Yu. Kardash, Svetlana V. Cherepanova and Andrei I. Boronin



20903

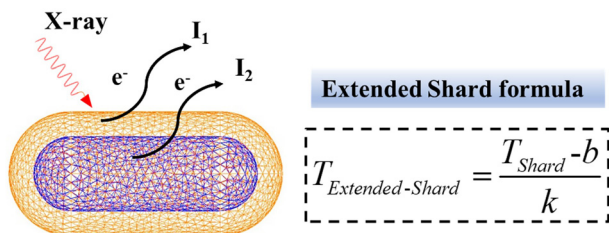
## In silico screening and computational evaluation of novel promising USP14 inhibitors targeting the palm–thumb pocket

Tianhao Wang, Jianbo Tong,\* Xing Zhang, Hao Luo, Lei Xu and Zhe Wang\*



## RESEARCH PAPERS

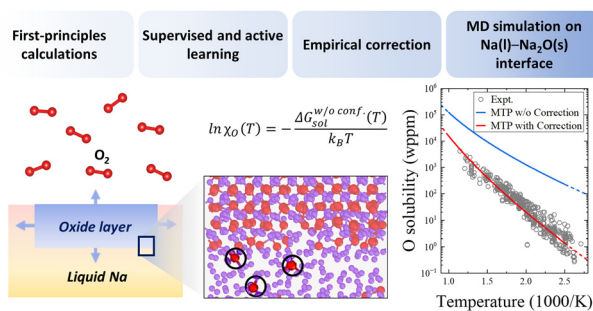
20917



### A theoretical characterization method for non-spherical core-shell nanoparticles by XPS

J. M. Gong, M. S. S. Khan, B. Da,\* H. Yoshikawa, S. Tanuma and Z. J. Ding\*

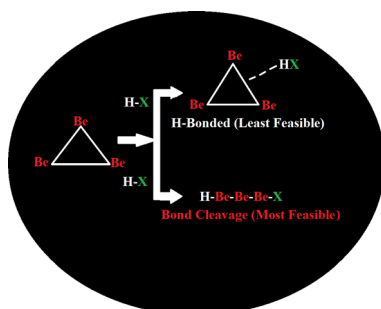
20933



### Temperature dependence of O solubility in liquid Na by atomistic simulation of Na(l)–Na<sub>2</sub>O(s) interfaces using corrected machine learning potential: a step towards simulating Na combustion

Chaeyeong Kim and Takuji Oda\*

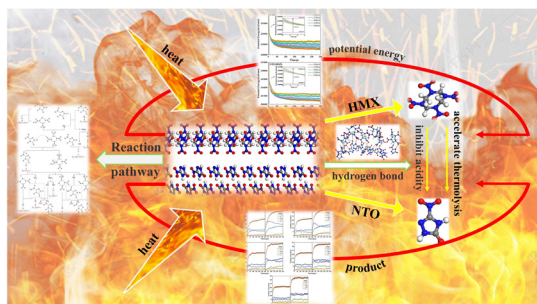
20947



### Three-membered beryllium ring, Be<sub>3</sub>: not just a hydrogen bond acceptor

Lakhya J. Mazumder and Ankur K. Guha\*

20951



### Multi-aspect simulation insight on thermolysis mechanism and interaction of NTO/HMX-based plastic-bonded explosives: a new conception of the mixed explosive model

Xiaofeng Yuan, Ying Huang, Shuhai Zhang,\* Ruijun Gou, Shuangfei Zhu and Qianjin Guo

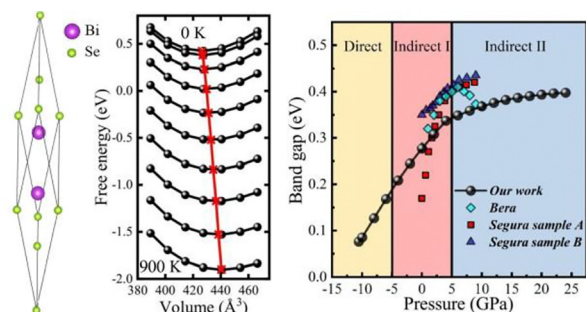


## RESEARCH PAPERS

20969

### Effects of pressure and temperature on topological electronic materials $X_2Y_3$ ( $X = \text{As, Sb, Bi}$ ; $Y = \text{Se, Te}$ ) using first-principles

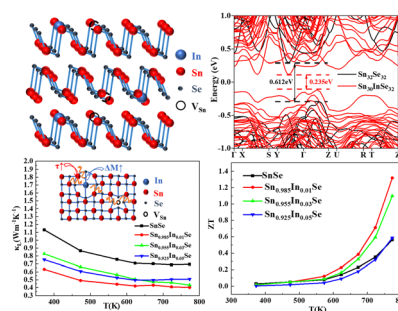
Le Fang, Chen Chen, Xionggang Lu\* and Wei Ren\*



20979

### Significantly improved thermoelectric performance of SnSe originating from collaborative adjustment between valence and conduction bands, mass fluctuations, and local strain

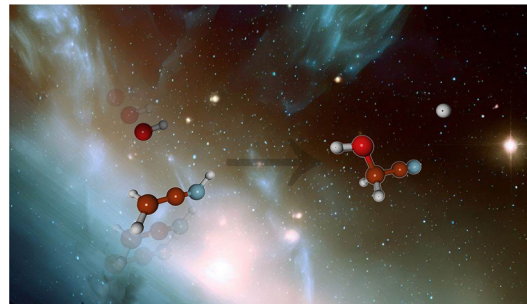
Shuai Wang, Hang Yuan, Chunhui Li, HongQuan Liu,\* Yi-jie Gu\* and YanFang Wang



20988

### Gas-phase formation of glycolonitrile in the interstellar medium

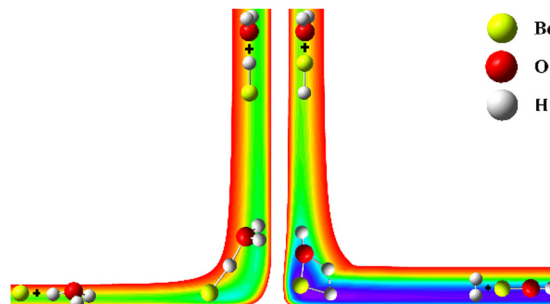
Luis Guerrero-Méndez, Anxo Lema-Saavedra, Elena Jiménez, Antonio Fernández-Ramos\* and Emilio Martínez-Núñez\*



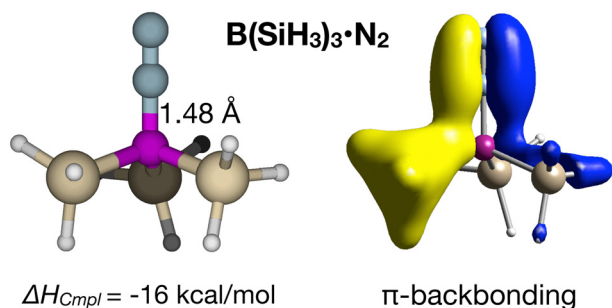
20997

### Theoretical studies on the kinetics and dynamics of the $\text{BeH}^+ + \text{H}_2\text{O}$ reaction: comparison with the experiment

Jiaqi Li, Zhao Tu, Haipan Xiang, Yong Li\* and Hongwei Song\*



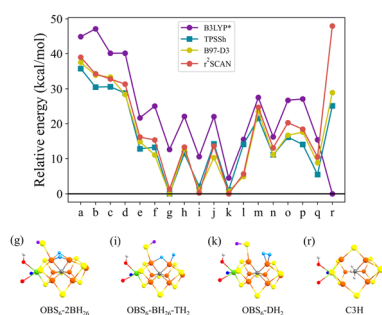
21006



**Anomalous  $\pi$ -backbonding in complexes between B(SiR<sub>3</sub>)<sub>3</sub> and N<sub>2</sub>: catalytic activation and breaking of scaling relations**

Tore Brinck\* and Suman Kalyan Sahoo

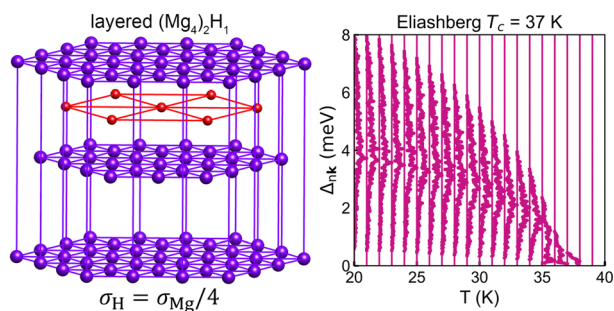
21020



**The E<sub>3</sub> state of FeMoco: one hydride, two hydrides or dihydrogen?**

Yunjie Pang and Ragnar Bjornsson\*

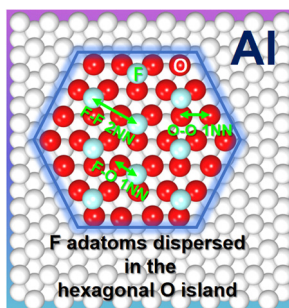
21037



**Enhancement for phonon-mediated superconductivity up to 37 K in few-hydrogen metal-bonded layered magnesium hydride under atmospheric pressure**

Yong He, Juan Du,\* Shi-ming Liu, Chong Tian, Min Zhang, Yao-hui Zhu, Hongxia Zhong, Xinqiang Wang and Jun-jie Shi\*

21045



**Morphology evolution of the aluminum surface in a fluorine-containing environment**

Pengqi Hai, Chao Wu,\* Xiangdong Ding\* and Yuanjie Li\*

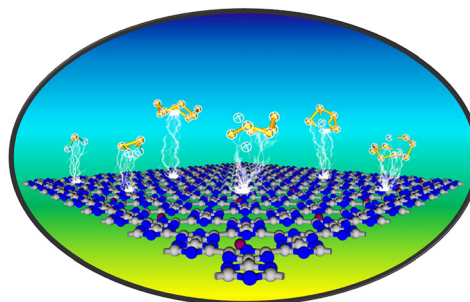


## RESEARCH PAPERS

21054

### Unveiling the anchoring and catalytic effect of Co@C<sub>3</sub>N<sub>3</sub> monolayer as a high-performance selenium host material in lithium–selenium batteries: a first-principles study

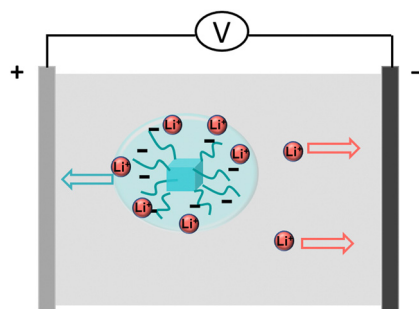
Shuwei Tang,\* Wentao Liu, Zehui Yang, Chenchen Liu, Shulin Bai, Jingyi Zhang and Dongming Luo



21065

### Lithium transference in electrolytes with star-shaped multivalent anions measured by electrophoretic NMR

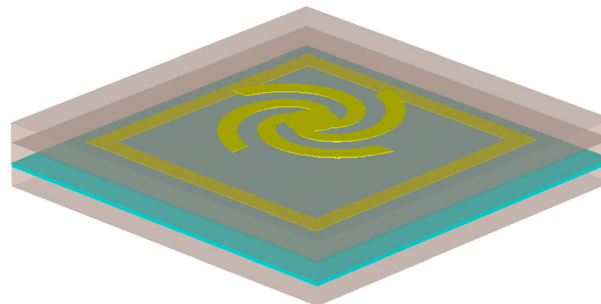
Saheli Chakraborty, David M. Halat, Julia Im, Darby T. Hickson, Jeffrey A. Reimer and Nitash P. Balsara\*



21074

### Polarization-insensitive electromagnetically induced transparency and its sensing performance based on spoof localized surface plasmons in vanadium dioxide-based terahertz metasurfaces

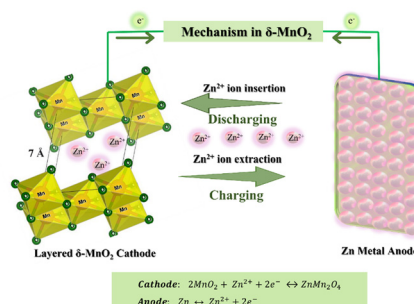
Mingming Chen\* and Xue-Xia Yang\*



21082

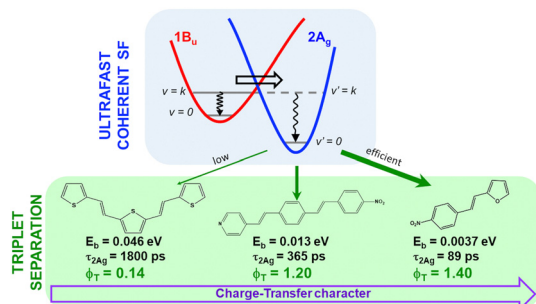
### A highly stable $\delta$ -MnO<sub>2</sub> cathode with superior electrochemical performance for rechargeable aqueous zinc ion batteries

Priya Yadav, Dimas Putro, Nisha Kumari, Jaekook Kim\* and Alok Kumar Rai\*



## RESEARCH PAPERS

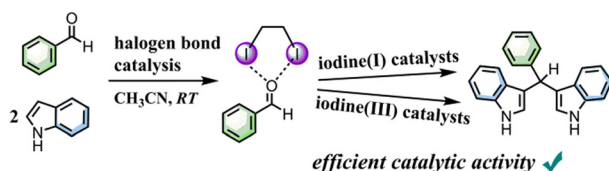
21089



### Unveiling the double triplet nature of the $2A_g$ state in conjugated stilbenoid compounds to achieve efficient singlet fission

Letizia Mencaroni, Martina Alebardi, Fausto Elisei, Irena Škorić, Anna Spalletti and Benedetta Carlotti\*

21100



### Iodine(I)-based and iodine(III)-based halogen bond catalysis on the Friedel–Crafts reaction: a theoretical study

Chang Zhao, Ying Li, Xiaoyan Li and Yanli Zeng\*

## CORRECTION

21109

### Correction: First-principles modeling of the highly dynamical surface structure of a $MoS_2$ catalyst with S-vacancies

Po-Yuan Wang, Bo-An Chen, Yu-Chi Lee and Cheng-chau Chiu\*

