

## IN THIS ISSUE

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### Cover

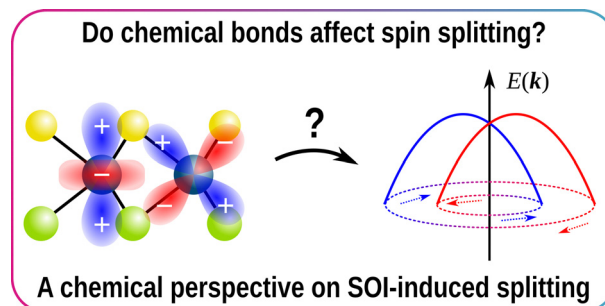
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*Phys. Chem. Chem. Phys.*,  
2023, 25, 30198.

## TUTORIAL REVIEW

30099

### Rashba effect: a chemical physicist's approach

Maciej J. Szary

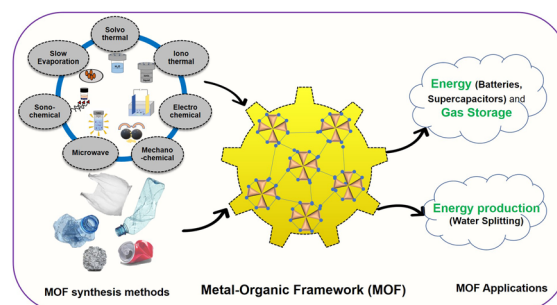


## REVIEW

30116

### Metal–organic frameworks (MOFs) for energy production and gaseous fuel and electrochemical energy storage applications

Mariyappan Shanmugam, Nithish Agamendran,  
Karthikeyan Sekar\* and Thillai Sivakumar Natarajan\*



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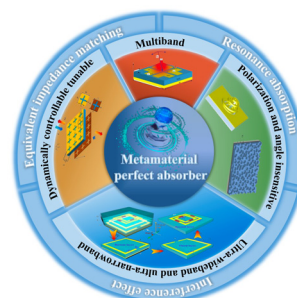


## PERSPECTIVES

30145

**Structures, principles, and properties of metamaterial perfect absorbers**

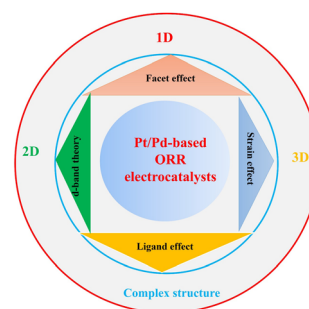
Chenxu Zhao, Huan Wang, Yanyan Bu, Hui Zou\* and Xiangfu Wang\*



30172

**Nanostructure engineering of Pt/Pd-based oxygen reduction reaction electrocatalysts**

Le Li,\* Xintong Ye, Qi Xiao, Qianyi Zhu, Ying Hu and Meijun Han

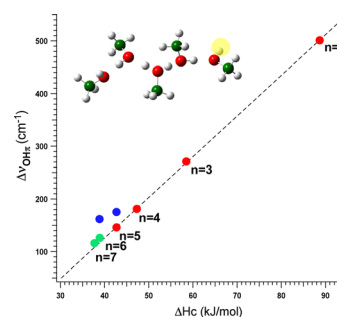


## COMMUNICATIONS

30188

**Experimental confirmation of the Badger–Bauer rule in the protonated methanol clusters: weak hydrogen bond formation as a measure of terminal OH acidity in hydrogen bond networks**

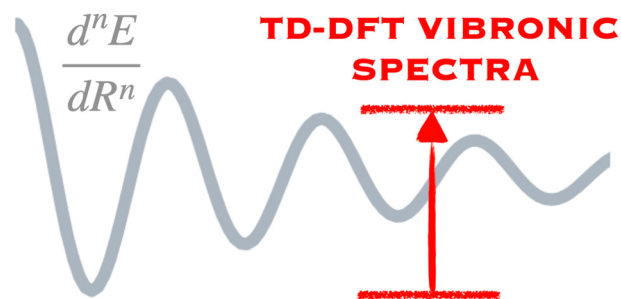
Takeru Kato and Asuka Fujii\*



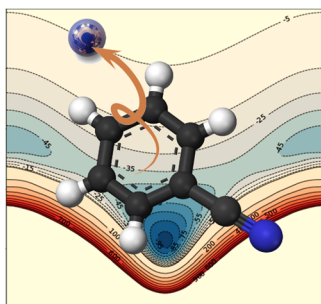
30193

**Pitfall in simulations of vibronic TD-DFT spectra: diagnosis and assessment**

Sebastian P. Sitkiewicz,\* Eduard Matito, Josep M. Luis\* and Robert Zalesny\*



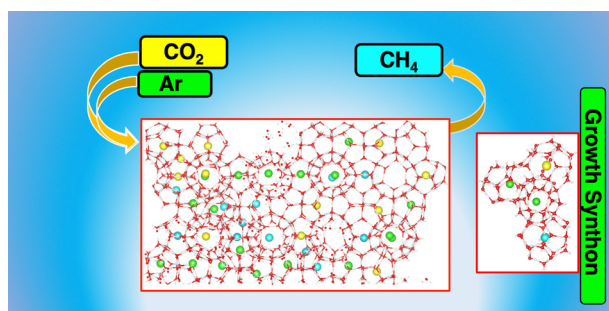
30198



### Towards the generation of potential energy surfaces of weakly bound medium-sized molecular systems: the case of benzonitrile–He complex

Eya Derbali, Yosra Ajili,\* Bilel Mehnen, Piotr S. Żuchowski, Dariusz Kędziera,\* Muneerah Mogren Al-Mogren, Nejm-Edine Jaidane and Majdi Hochlaf\*

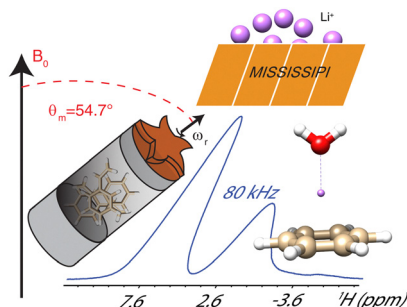
30211



### Carbon dioxide sequestration in natural gas hydrates – effect of flue and noble gases

Manju Sharma\* and Satyam Singh

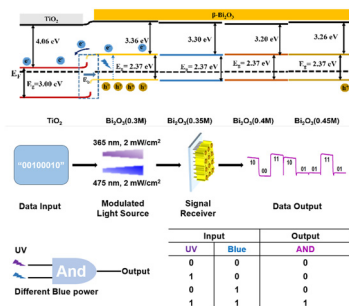
30223



### Regulating polystyrene glass transition temperature by varying the hydration levels of aromatic ring/Li<sup>+</sup> interaction

Sze Yuet Chin, Yunpeng Lu, Weishuai Di, Kai Ye, Zihan Li, Chenlu He, Yi Cao, Chun Tang and Kai Xue\*

30228



### Improved performance of UV-blue dual-band Bi<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> photodetectors and application of visible light communication with UV light encryption

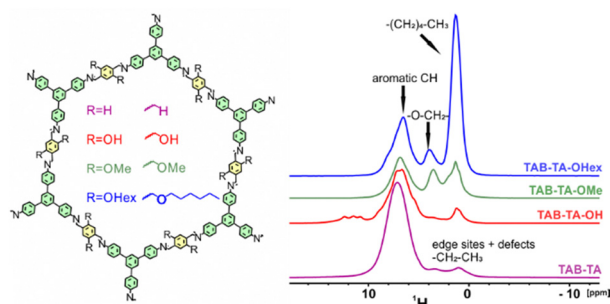
Qin Zheng, Jianping Xu,\* Shaobo Shi, Jing Chen, Jianghua Xu, Lina Kong, Xiaosong Zhang and Lan Li



30237

## High-field and fast-spinning $^1\text{H}$ MAS NMR spectroscopy for the characterization of two-dimensional covalent organic frameworks

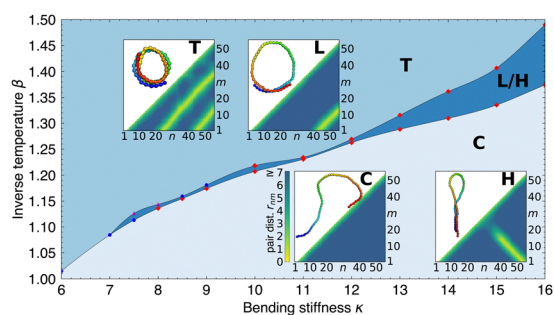
Nikolaj Lopatik, Ankita De, Silvia Paasch, Andreas Schneemann and Eike Brunner\*



30246

## Secondary-structure phase formation for semiflexible polymers by bifurcation in hyperphase space

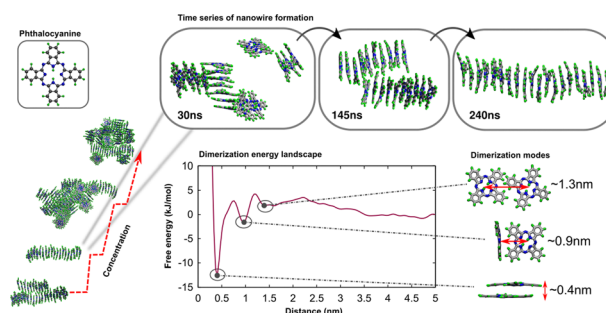
Dilimulati Aierken\* and Michael Bachmann\*



30259

## Molecular mechanisms underlying nanowire formation in pristine phthalocyanine

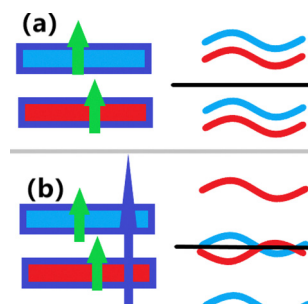
Aadil Pinjari, Deepashri Saraf\* and Durba Sengupta\*



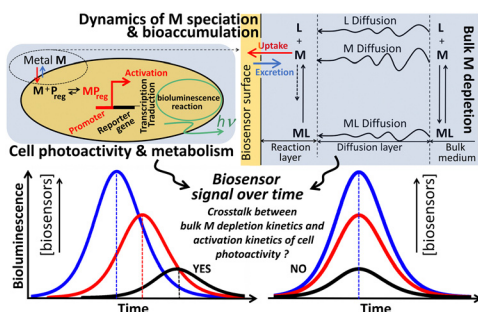
30269

## Electric-field induced half-metallic properties in an experimentally synthesized CrSBr monolayer

Hao-Tian Guo, San-Dong Guo\* and Yee Sin Ang



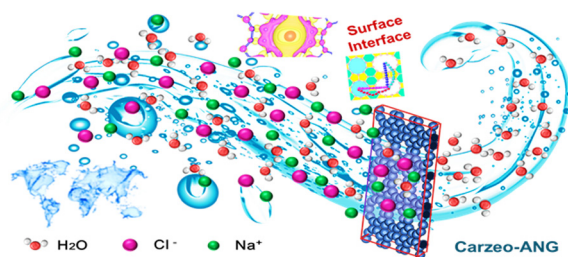
30276



### Kinetics of metal detection by luminescence-based whole-cell biosensors: connecting biosensor response to metal bioavailability, speciation and cell metabolism

Jérôme F. L. Duval,\* Lorenzo Maffei, Eva Delatour, Marie Zaffino and Christophe Pagnout

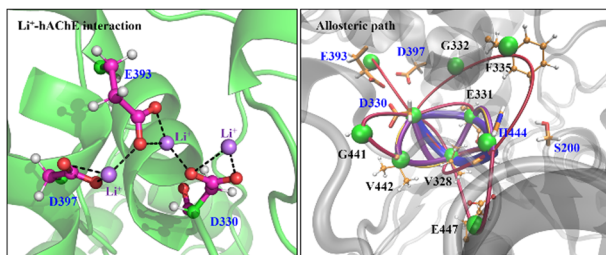
30296



### Surface/interfacial transport through pores control desalination mechanisms in 2D carbon-based membranes

Xiaoyang Zhao, Kun Meng,\* Yutao Niu, Sen Ming, Ju Rong, Xiaohua Yu and Yannan Zhang

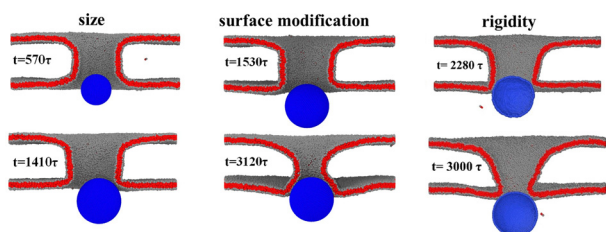
30308



### Selective modulation of alkali metal ions on acetylcholinesterase

Xia Mu, Shengwei Yuan, Dinglin Zhang, Rui Lai, Chenyi Liao\* and Guohui Li\*

30319



### Probe the nanoparticle–nucleus interaction via coarse-grained molecular model

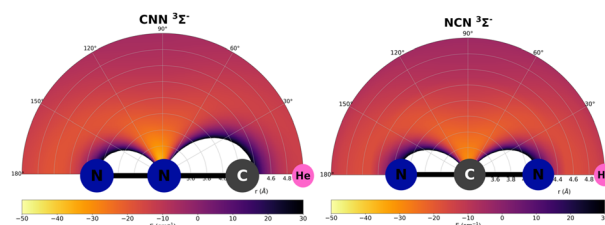
LiuYang Zhang, Ning Liu\* and Xianqiao Wang



30330

### Collision-induced state-changing rate coefficients for cyanogen backbones $\text{NCN } ^3\Sigma^-$ and $\text{CNN } ^3\Sigma^-$ in astrophysical environments

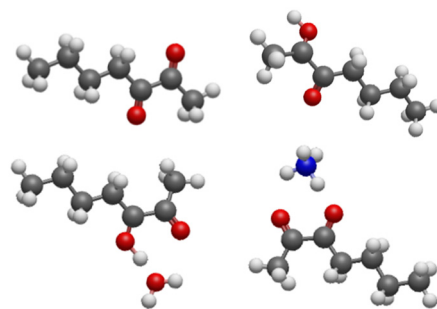
Lola González-Sánchez, Ersin Yurtsever, Jorge Alonso de la Fuente, Cristina Sanz-Sanz, Roland Wester and Francesco A. Gianturco\*



30343

### Gas phase $\text{H}^+$ , $\text{H}_3\text{O}^+$ and $\text{NH}_4^+$ affinities of oxygen-bearing volatile organic compounds; DFT calculations for soft chemical ionisation mass spectrometry

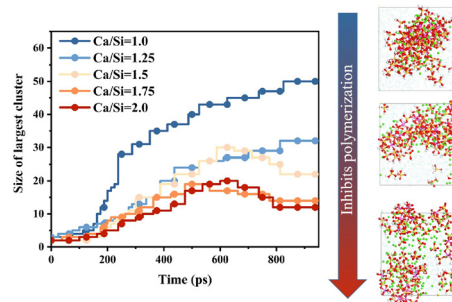
Maroua Omezzine Gnioua, Anatolii Spesyvyi and Patrik Španěl\*



30349

### The inhibitory effect of excess calcium ions on the polymerization process of calcium aluminate silicate hydrate (CASH) gel

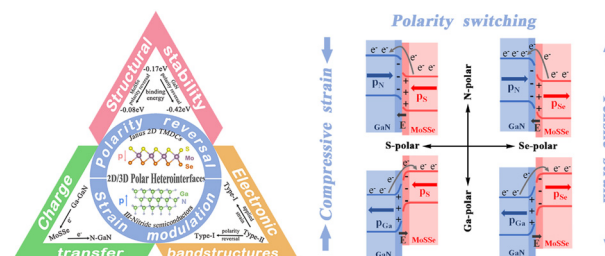
Dongshuai Hou, Mengqi Sun, Muhan Wang, Zheng Chen, Xinpeng Wang, Yue Zhang and Pan Wang\*



30361

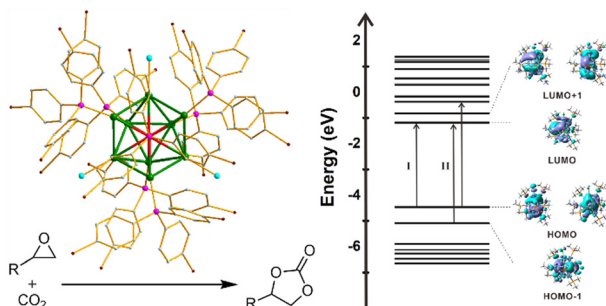
### Polarity reversal and strain modulation of Janus $\text{MoSSe}/\text{GaN}$ polar semiconductor heterostructures

Delin Kong, Feng Tian, Yingying Xu, Shaoqun Zhu, Zetong Yu, Lefeng Xiong, Peipei Li, Huiyun Wei, Xinhe Zheng\* and Mingzeng Peng\*



## RESEARCH PAPERS

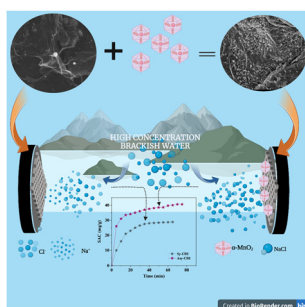
30373



### One-step preparation of Pt/Ag nanoclusters for CO<sub>2</sub> transformation

Meng Wang, Simin Li, Xiongfai Tang, Dongjie Zuo, Yanyuan Jia,\* Shuo Guo, Zong-Jie Guan\* and Hui Shen\*

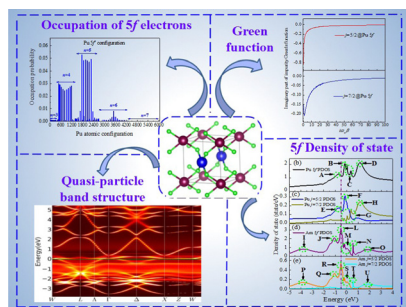
30381



### Solar reduced graphene oxide decorated with manganese dioxide nanostructures for brackish water desalination using asymmetric capacitive deionization

Shreerang D. Datar, Nitish Kumar, Vrushali Sawant, Noora Shaikh and Neetu Jha\*

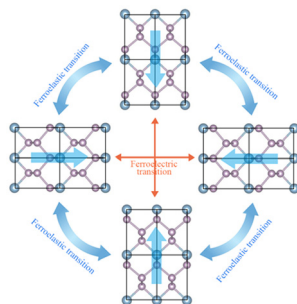
30391



### Electron correlation and relativistic effects on the electronic properties of a plutonium and americium mixed oxide (PuAmO<sub>4</sub>): from single-particle approximation to dynamical mean-field theory

Ru-song Li,\* Jin-tao Wang, Zhi-yong Liu, Xiao-hua Zhou, Ze-lin Cao and Zheng Xie\*

30405



### Auxetic and multiferroic MP<sub>5</sub> (M = Al, Ga): a novel 2D material with negative Poisson's ratio and high anisotropic carrier mobility

Qingwen Lan and Changpeng Chen\*



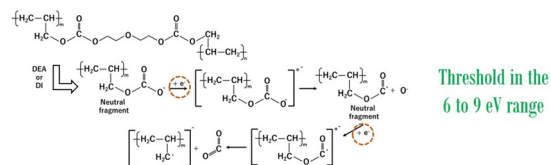
## RESEARCH PAPERS

30412

### Revealing the mechanism of damage to the carbonate ester in PADC polymeric nuclear track detector using low-energy electron stimulated desorption

Tamon Kusumoto, Michel Fromm,\* Pierre Cloutier, Andrew D Bass, Léon Sanche and Satoshi Kodaira

The key to understanding the mechanisms of molecular damage by radiation is the number and energy of electrons interacting with fundamental molecular units.

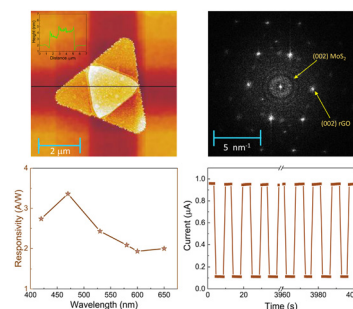


The present results indicate that desorbed  $O^-$  signal derives in unirradiated films, from the oxygen atom adjacent to the carbonyl bond.

30419

### Photogating induced high sensitivity and speed from heterostructure of few-layer $MoS_2$ and reduced graphene oxide-based photodetector

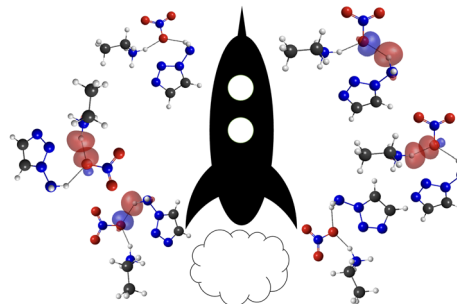
Chayan Das, Ashok Kumar, Suresh Kumar, Neha V. Dambhare, Mahesh Kumar, Arup K. Rath and Satyajit Sahu\*



30428

### Intermolecular interactions in clusters of ethylammonium nitrate and 1-amino-1,2,3-triazole

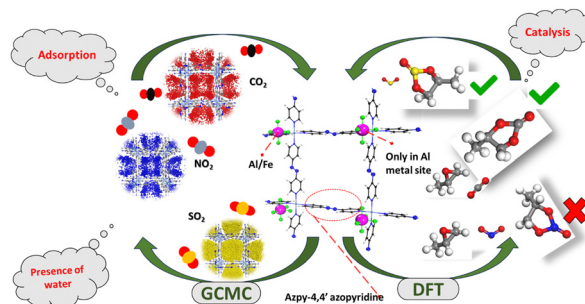
Shinae Kim,\* Justin A. Conrad, Garrett M. Tow, Edward J. Maginn, Jerry A. Boatz and Mark S. Gordon\*



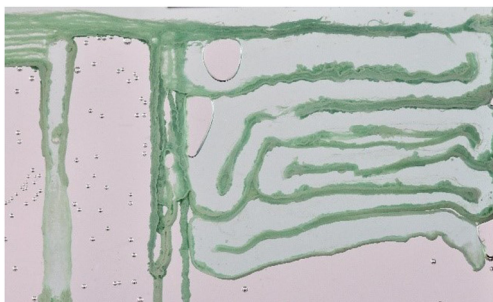
30458

### Prediction of the capture and utilization of atmospheric acidic gases by azo-based square-pillared fluorinated MOFs

D. Muthukumar, Athulya S. Palakkal and Renjith S. Pillai\*



30469

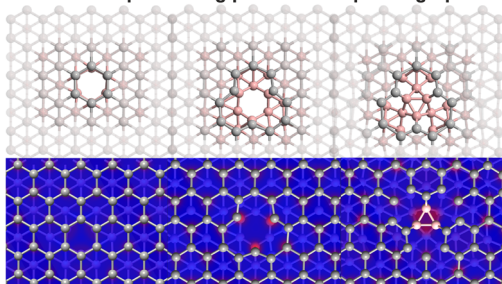


### A microfluidic labyrinth self-assembled by a chemical garden

Sergio Testón-Martínez,\* Teresa Huertas-Roldán, Pamela Knoll, Laura M. Barge, C. Ignacio Sainz-Díaz and Julyan H. E. Cartwright\*

30477

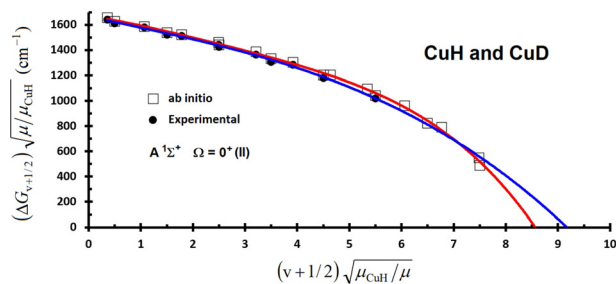
### The minimal perforating pores in borophene-graphene



### On point perforating defects in bilayer structures

Aleksey I. Kochaev, Vladimir V. Efimov, Savas Kaya, Roberto Flores-Moreno, Konstantin P. Katin and Mikhail M. Maslov\*

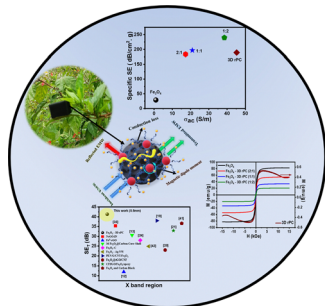
30488



### Spin-orbit coupling in low-lying electronic states of CuH

Zeinab Mohammadian and Alireza Shayesteh\*

30501



### High-performance EMI shielding effectiveness of Fe<sub>3</sub>O<sub>4</sub>-3D rPC nanocomposites: a systematic optimization in the X-band region

Theertharaman Govindasamy, Nibin Kolanjikombil Mathew, Vinaya Kumar Asapu, Vijayshankar Asokan, Venkatachalam Subramanian and Balakumar Subramanian\*

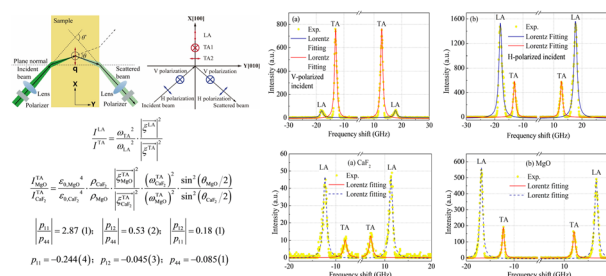


## RESEARCH PAPERS

30516

## Photoelasticity of a MgO single crystal from polarized Brillouin scattering spectroscopy

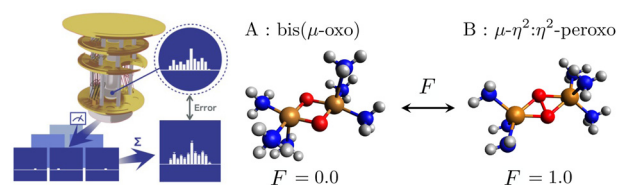
YongQuan Wu,\* ZhengPing Bao and JingLin You



30525

## Statistical errors in reduced density matrices sampled from quantum circuit simulation and the impact on multireference perturbation theory

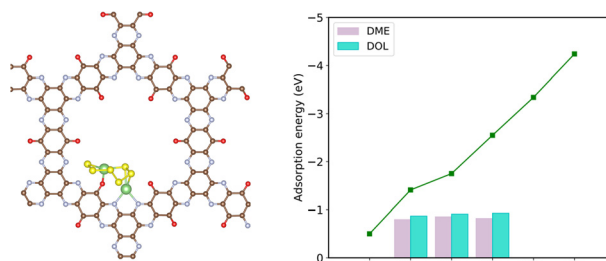
Soichiro Nishio, Yuki Oba and Yuki Kurashige\*



30536

## A nitrogen-rich two dimensional covalent organic framework with multiple carbonyls as a highly efficient anchoring material for lithium–sulfur batteries

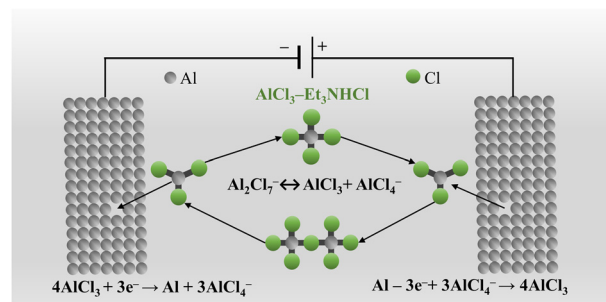
Priya Das and Pranab Sarkar\*



30543

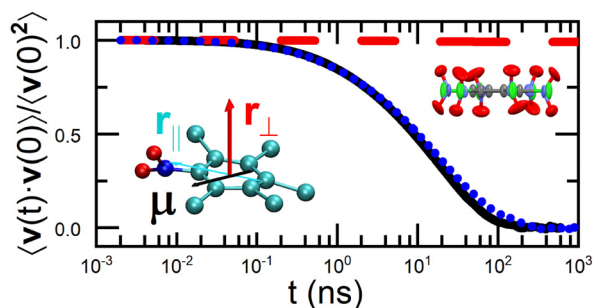
## Electrochemical behavior of aluminum in triethylamine hydrochloride–aluminum chloride ionic liquid

Alexey V. Borozdin,\* Peter Yu. Shevelin, Vladimir A. Elterman and Liudmila A. Yotshina



## RESEARCH PAPERS

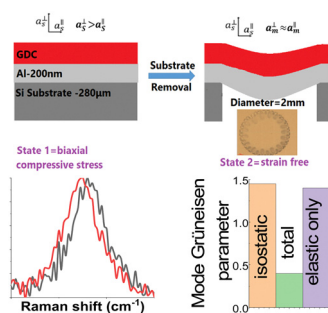
30553



### Dynamics and local ordering of pentachloronitrobenzene: a molecular-dynamics investigation

Jonathan F. Gebbia,\* Andrés Henao Aristizabal, Philippe Negrier, David Aguilà, Josep Lluís Tamarit and Luis Carlos Pardo

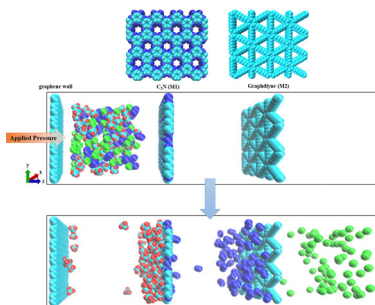
30563



### The elastic component of anisotropic strain dominates the observed shift in the $F_{2g}$ Raman mode of anelastic ceria thin films

Daniel Freidzon, Olga Kraynis, Ellen Wachtel, Igor Lubomirsky\* and Tsachi Livneh\*

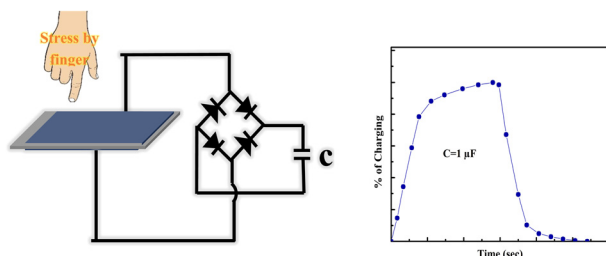
30572



### Highly efficient helium purification through a dual-membrane system: insights from molecular dynamics simulations

Siamak Pakdel, Hamid Erfan-Niya,\* Jafar Azamat and Amir Hasanzadeh

30583



### A self-powered mechanical energy harvester based on $\text{CH}_3\text{NH}_3\text{PbI}_3$ doped P(VDF-HFP)/PANI composite films

Priti Sundar Barman, Samiran Garain\* and Prakriti Adhikary\*

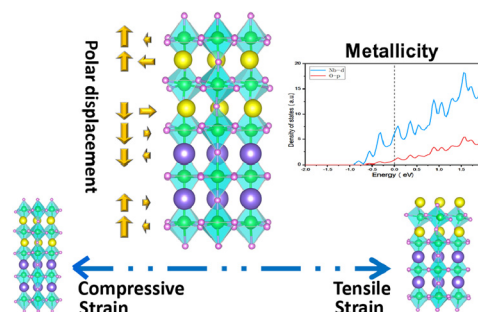


## RESEARCH PAPERS

30596

Polar metals in strain-engineered  $\text{KNbO}_3/\text{CaNbO}_3$  superlattices: a first-principles study

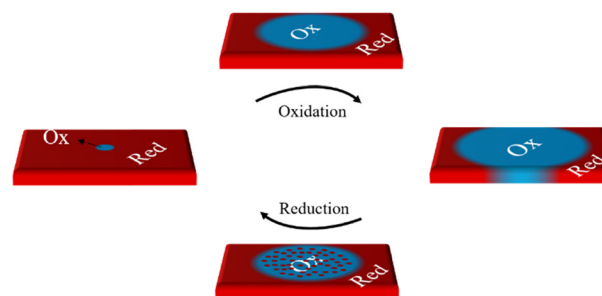
Qihang Liang, Fawei Zheng and Menglei Li\*



30606

## Autocatalytic solid-state electrochemical reactions: a non-linear kinetic theory of batteries

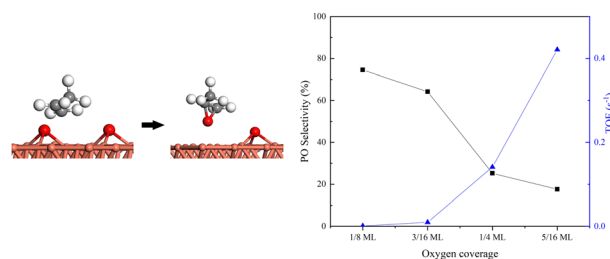
Keyvan Malaie



30612

## Investigation of the oxygen coverage effect on the direct epoxidation of propylene over copper through DFT calculations

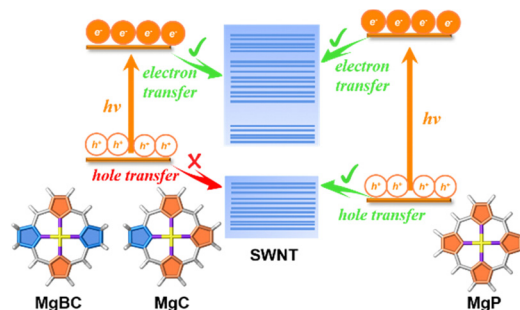
Ben Sun and Gui-Chang Wang\*



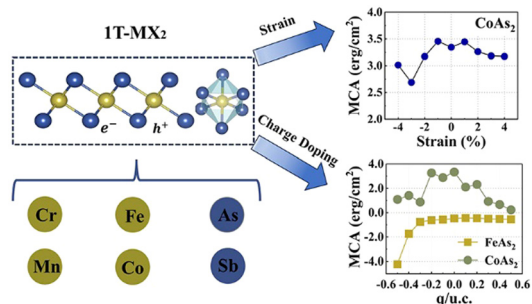
30627

## Mechanistic insights into photoinduced energy and charge transfer dynamics between magnesium-centered tetrapyrroles and carbon nanotubes

Jia-Ning Zhou, Ke-Qin Cheng, Xiaolong Zhang, Shubin Yang, Jie Liu, Wenzuo Li, Qingzhong Li, Juan Han,\* Xiao-Ying Xie\* and Ganglong Cui



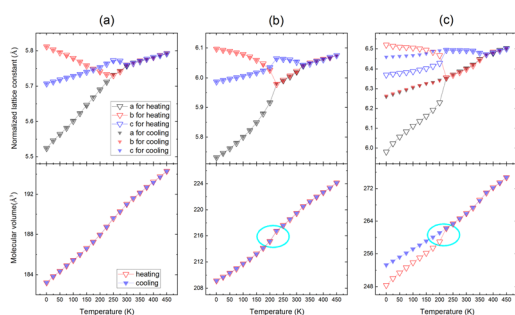
30636



### Intrinsic ferromagnetism in two-dimensional 1T-MX<sub>2</sub> monolayers with tunable magnetocrystalline anisotropy

Yonghao Wang, Zesen Lei, Meng Guo, Qilong Sun,\*  
Cui Jin, Ruishan Tan and Ying Dai\*

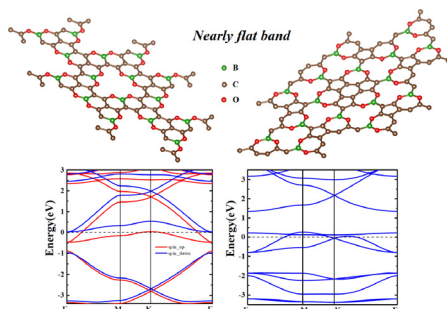
30644



### Investigation of phase transition, mechanical behavior and lattice thermal conductivity of halogen perovskites using machine learning interatomic potentials

Yongbo Shi, Yuanyuan Chen, Haikuan Dong,\*  
Hao Wang and Ping Qian\*

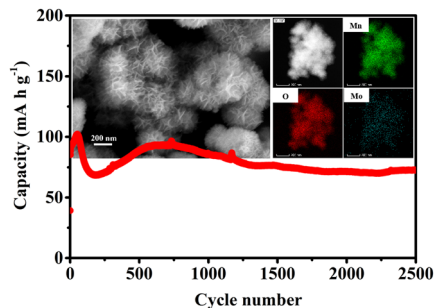
30656



### New two-dimensional flat band materials: B<sub>3</sub>C<sub>11</sub>O<sub>6</sub> and B<sub>3</sub>C<sub>15</sub>O<sub>6</sub>

Jialuo Dong, Pan Zhou,\* Yuzhong Hu and Lizhong Sun\*

30663



### Inhibition of phase transition from $\delta$ -MnO<sub>2</sub> to $\alpha$ -MnO<sub>2</sub> by Mo-doping and the application of Mo-doped MnO<sub>2</sub> in aqueous zinc-ion batteries

Yubin Liu,\* Wenjie Chen, Jingjing Su, Xiaojing Zhao and Xiaoyang Pan

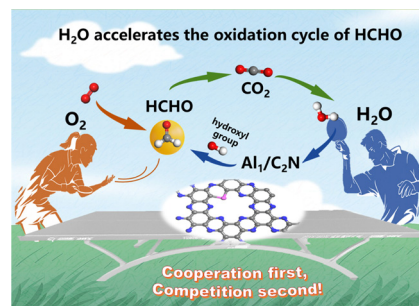


## RESEARCH PAPERS

30670

### Unveiling the intrinsic role of water in the catalytic cycle of formaldehyde oxidation: a comprehensive study integrating density functional theory and microkinetic analysis

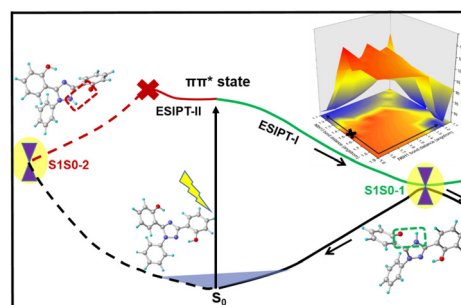
Qianyu Li, Wenlang Li, Jiachun Cao, Junhui Zhou, Didi Li and Zhimin Ao\*



30679

### Excited-state relaxation mechanisms of 2,2'-(1-phenyl-1H-1,2,4-triazole-3,5-diyl)diphenol: single- or double-proton transfer?

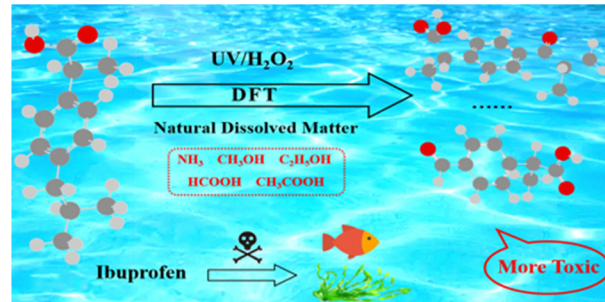
Jiahui Wu, Jihuan He, Wei Wang, Xiaohang Chen and Shu-Hua Xia\*



30687

### New insights into the degradation mechanism of ibuprofen in the UV/H<sub>2</sub>O<sub>2</sub> process: role of natural dissolved matter in hydrogen transfer reactions

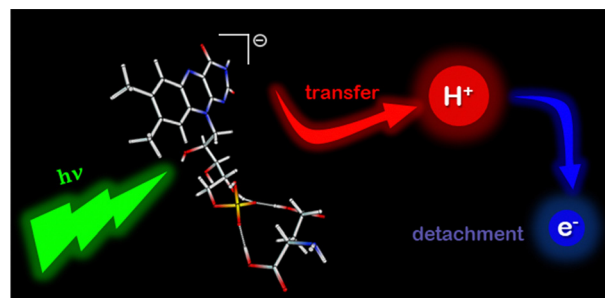
Zhezhen Ding, Jiahui Zhang, Timing Fang, Guohui Zhou, Xiao Tang, Yan Wang and Xiaomin Liu\*



30697

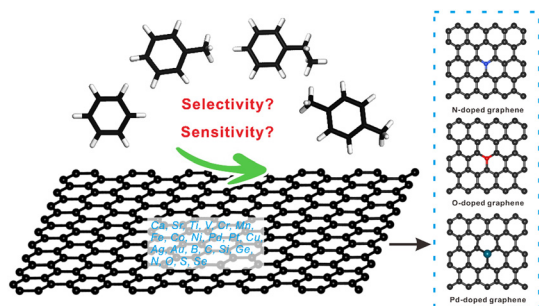
### Photodissociative decay pathways of the flavin mononucleotide anion and its complexes with tryptophan and glutamic acid

Kelechi O. Uleanya, Cate S. Anstöter and Caroline E. H. Dessent\*



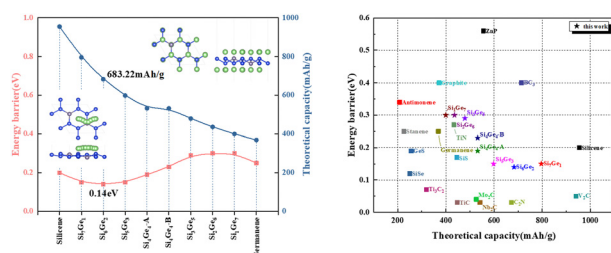
## RESEARCH PAPERS

30708

**BTEX sensing potential of elemental-doped graphene: a DFT study**

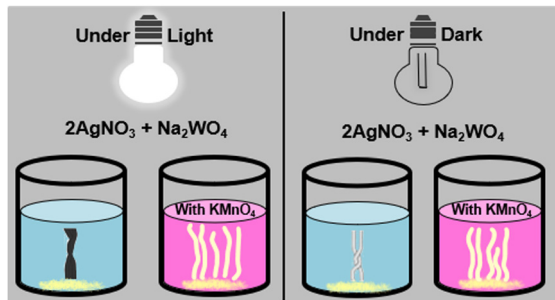
Hongping Zhang,\* Run Zhang, Shuchun Hu, Kun Yang, Qingyuan Wang, Huilong Dong, Yuxiang Ni and Wei Feng

30716

**The effect of Ge doping concentration on the electrochemical performance of silicene anode for lithium-ion batteries: a first-principles study**

Jun Song,\* Mingjie Jiang, Jodie A. Yuwono, Sailin Liu, Jingxiu Wang, Qi Zhang, Yuhui Chen, Jun Zhang, Xuehong Wu and Juanfang Liu\*

30727

**Light-modulated colour transformation in highly intertwined vertically growing silver tungstate tubes**

Vipul Kirtikumar Patel and Balanagulu Busupalli\*

## CORRECTION

30735

**Correction: The solution structures and relative stability constants of lanthanide–EDTA complexes predicted from computation**

Ravi D. O'Brien, Thomas J. Summers, Danil S. Kaliakin and David C. Cantu\*

