

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

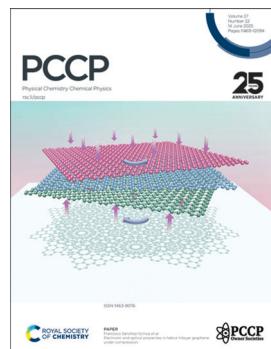
### IN THIS ISSUE

ISSN 1463-9076 CODEN PPCFQ 27(22) 11469–12094 (2025)



#### Cover

See Malay Kumar Rana et al., pp. 11530–11540.  
Image reproduced by permission of Malay Kumar Rana from *Phys. Chem. Chem. Phys.*, 2025, 27, 11530.



#### Inside cover

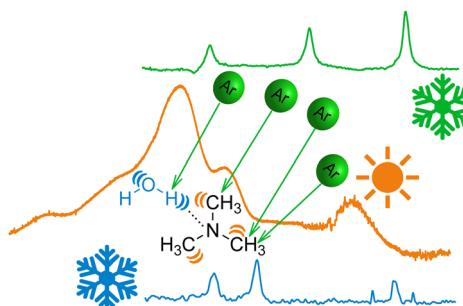
See Francisco Sánchez-Ochoa et al., pp. 11541–11550.  
Image reproduced by permission of Francisco Sánchez-Ochoa from *Phys. Chem. Chem. Phys.*, 2025, 27, 11541.

### COMMUNICATIONS

11487

#### OH-stretching dynamics in trimethylamine monohydrate: what can we learn from three different direct absorption spectra?

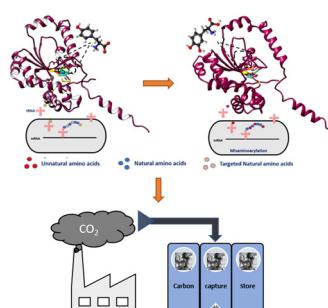
Taija L. Fischer, Casper V. Jensen, Eaindra Lwin, Dhritabrata Pal, Henrik G. Kjaergaard\* and Martin A. Suhm\*



11492

#### Intrinsic proton transfer activation of L-DOPA encoded carbonic anhydrase for efficient CO<sub>2</sub> sequestration

Ashokraj Sundarapandian, Prem Suresh, Sisila Valappil and Niraikulam Ayyadurai\*





# RSC Applied Interfaces

GOLD  
OPEN  
ACCESS

## Interfacial and surface research with an applied focus

### Interdisciplinary and open access



[rsc.li/RSCApplInter](http://rsc.li/RSCApplInter)

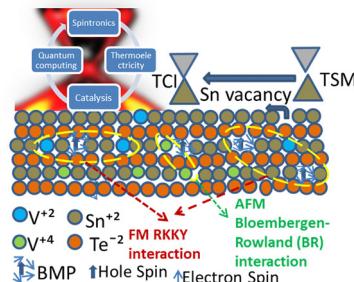
Fundamental questions  
Elemental answers

## RESEARCH PAPERS

11499

**Study of proximity-coupled magnetic anisotropy in V-doped SnTe using spin resonance and magnetic measurements**

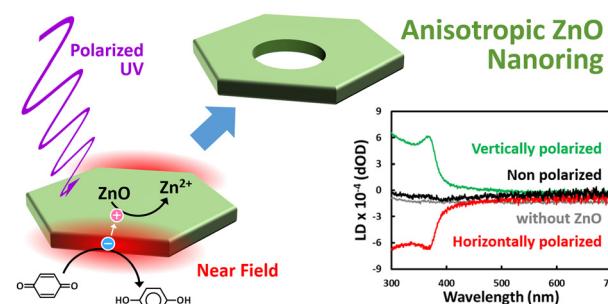
Subhadip Ghosh\* and Sanjeev Kumar Srivastava



11512

**Optically anisotropic ZnO nanorings fabricated using near-field photoelectrochemistry**

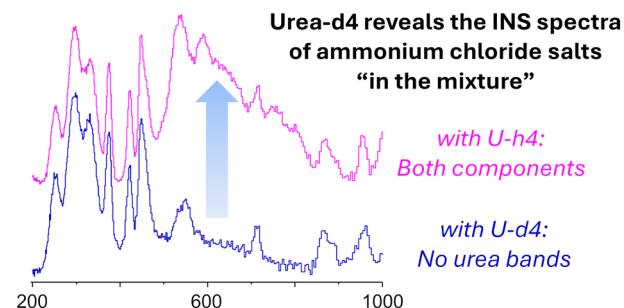
Yuki Oba, Seung Hyuk Lee and Tetsu Tatsuma\*



11518

**Decoding disorder: unravelling entropy effects in deep eutectic systems with neutron spectroscopy**

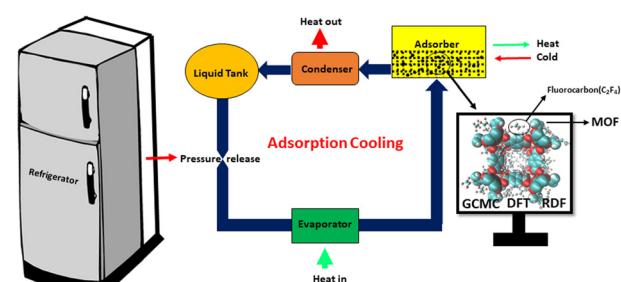
Rafael A. F. Serrano, Catarina F. Araújo, Paulo Ribeiro-Claro, Pedro D. Vaz, Svetmir Rudić, João A. P. Coutinho and Mariela M. Nolasco\*



11530

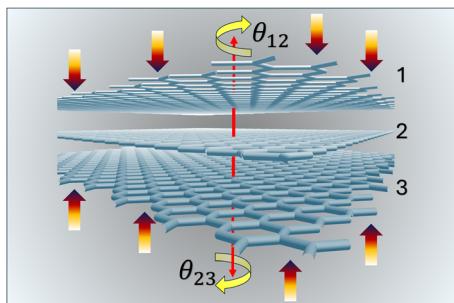
**Investigation of metal–organic frameworks and fluorocarbon refrigerants promising for adsorption cooling systems**

Dipankar Singha, Debansh Mohapatra and Malay Kumar Rana\*



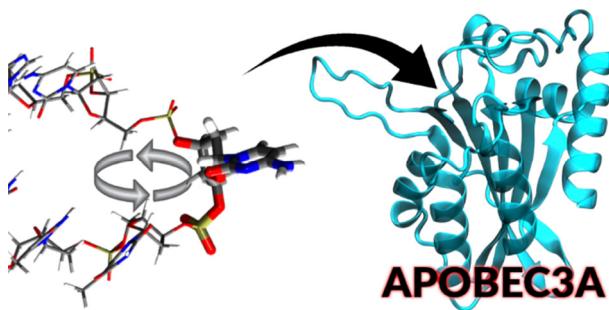
## RESEARCH PAPERS

11541

**Electronic and optical properties in helical trilayer graphene under compression**

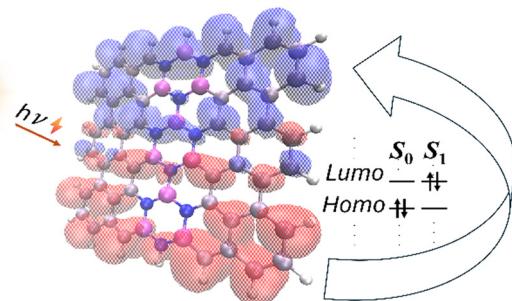
Ossiel Aguilar-Spíndola, Alberto Rubio-Ponce, Florentino López-Urías and Francisco Sánchez-Ochoa\*

11551

**DNA hairpin base-flipping dynamics drives APOBEC3A recognition and selectivity**

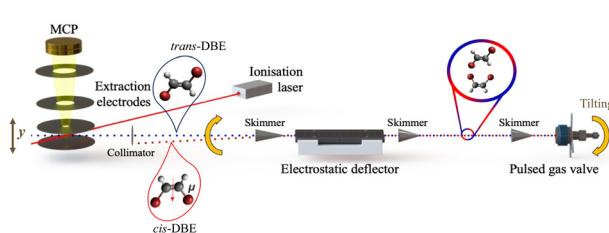
Mark A. Hix, A. G. Pramoda Sahankumari, Ashok S. Bhagwat and Alice R. Walker\*

11558

**Charge transfer within excited states of boron/nitrogen doped polycyclic aromatic hydrocarbons**

Luan G. F. dos Santos, Julio C. V. Chagas, Reed Nieman, Adelia J. A. Aquino, Francisco B. C. Machado\* and Hans Lischka\*

11570

**Isomer-selective dissociation dynamics of 1,2-dibromoethene ionised by femtosecond-laser radiation**

Amit Mishra, Junggil Kim, Sang Kyu Kim\* and Stefan Willitsch\*

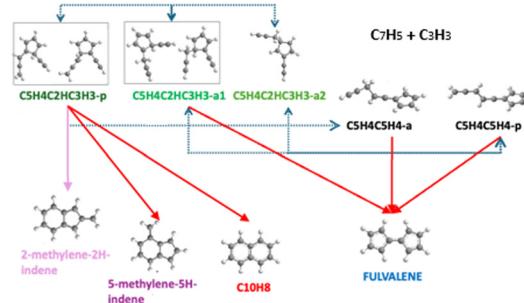


## RESEARCH PAPERS

11577

**Rate constants of the fulvenallenyl recombination with propargyl and its role in PAH formation: a theoretical and kinetic modeling study**

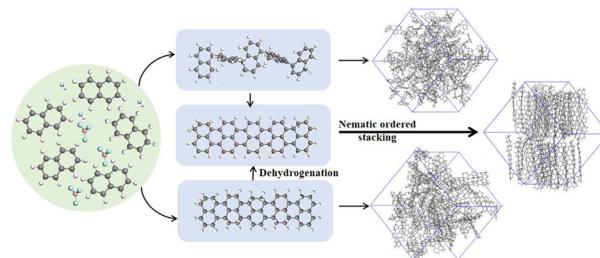
Alexander N. Morozov, Luna Pratali Maffei\* and Alexander M. Mebel\*



11597

**Research on the reaction mechanism and molecular stacking of acid catalyzed naphthalene to prepare mesophase pitches**

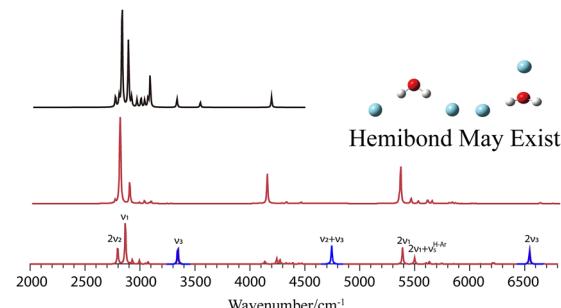
Xi Fan,\* Qiang Ren and Wen-kai Wei



11609

**Theoretical study on the structures and vibrational spectra of  $(H_2O-Ar_n)^+$ ,  $n = 1, 2$ : formation of a hemi-bond of water radical cation**

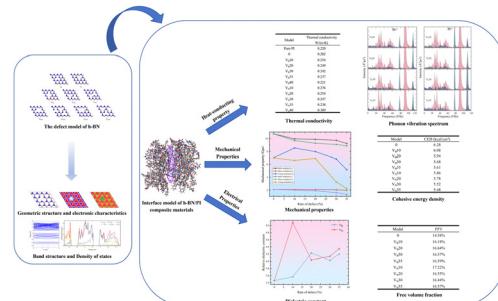
Jing-Min Liu,\* Qian-Rui Huang, Chih-Kai Lin and Jer-Lai Kuo\*



11617

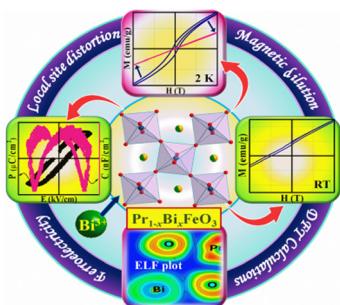
**Influence mechanism of vacancy defect effects on the intrinsic electronic properties of h-BN and the thermodynamic and dielectric properties of h-BN/PI interfaces**

Lujia Wang, Guangliang Liu, Wenyu Ye, Jianwen Zhang\* and Dingyu Bao



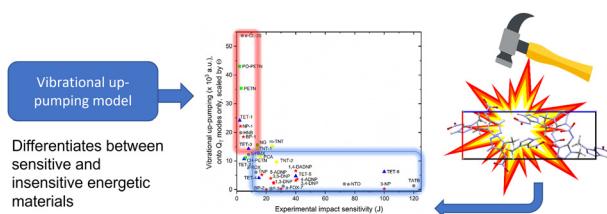
## RESEARCH PAPERS

11628

**Implications of magnetic dilution of  $\text{PrFeO}_3$  with  $\text{Bi}^{3+}$  on its dielectric and magnetic properties**

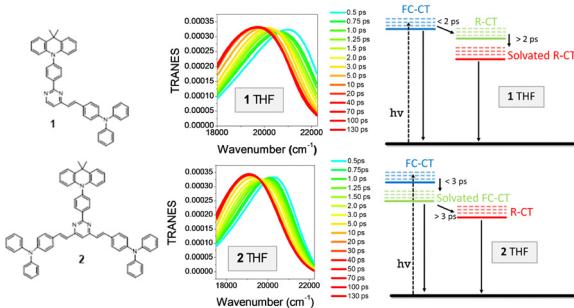
Shivangi Rao, Subhajit Sau, V. Kanchana, G. Vaitheswaran\* and Rajamani Nagarajan\*

11640

**Predicting impact sensitivities for an extended set of energetic materials via the vibrational up-pumping model: molecular-based structure–property relationships identified**

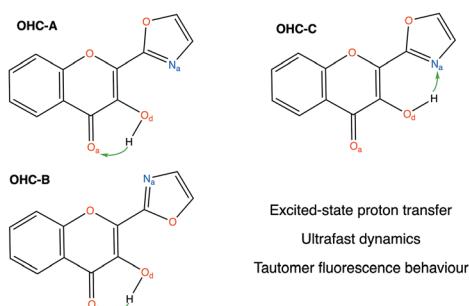
Jack M. Hemingway, Heather M. Quayle, Cian Byrne, Colin R. Pulham, Subrata Mondal, Adam A. L. Michalchuk\* and Carole A. Morrison\*

11649

**The role of branching in the ultrafast dynamics and two-photon absorption of two pyrimidine push–pull molecules**

Alexandros Katsidas, Michaela Fecková, Filip Bureš, Sylvain Achelle and Mihalis Fakis\*

11659

**Excited state proton transfer in 2-(oxazol-2-yl)-3-hydroxychromone**

Dipangkali Sarma and Sai G. Ramesh\*

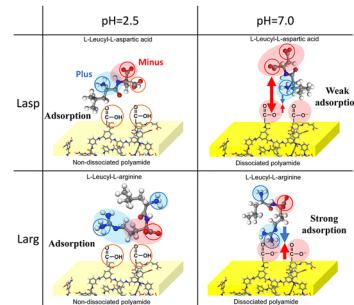


## RESEARCH PAPERS

11673

**Molecular simulations and an experimental study of the oligopeptide-mediated fouling mechanisms of polyamide reverse-osmosis membranes**

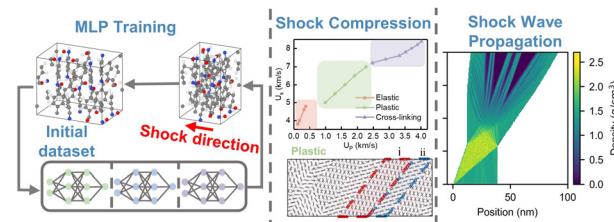
Ken Kinooka, Keizo Nakagawa, Hideto Matsuyama, Yu Fujimura, Takahiro Kawakatsu and Tomohisa Yoshioka\*



11684

**Machine-learning molecular dynamics simulations of shock response and spallation behavior in PPTA crystals**

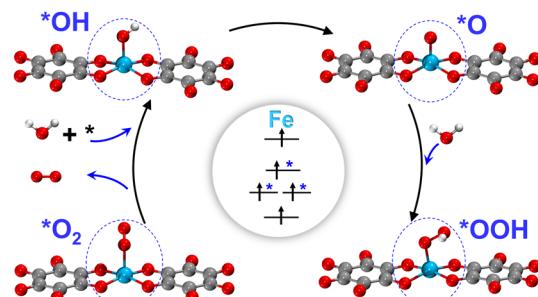
Lei Liu, Jingfu Shi, Di Song and Changqing Miao\*



11700

**Spin: an essential factor in advancing the oxygen evolution reaction on 2D Fe-MOF**

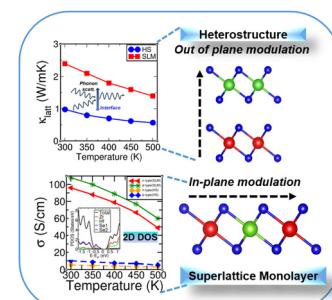
Erdembayalag Batsaikhan, Michitoshi Hayashi\* and Batjargal Sainbileg\*



11708

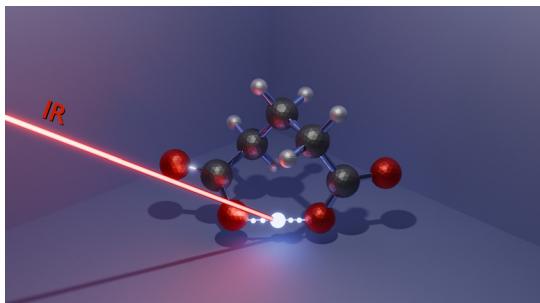
**Identifying key descriptors in  $\text{ZrSe}_2/\text{HfSe}_2$ -based heterostructures and superlattices for enhancing thermoelectric performance**

Tanu Choudhary, Satarupa Banik, Jipin Peter and Raju K. Biswas\*



## RESEARCH PAPERS

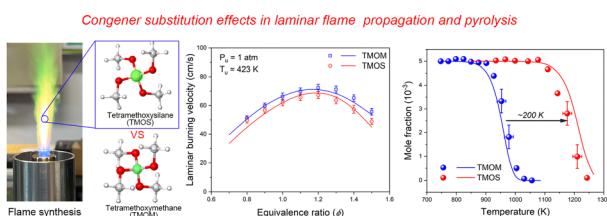
11725



## Intramolecular proton bonding in aliphatic dicarboxylate anions: dynamic conformational landscapes and spectral signatures

Marcos de Lucas, Juan R. Avilés-Moreno, Giel Berden, Jonathan Martens, Jos Oomens, Francisco Gámez\* and Bruno Martínez-Haya\*

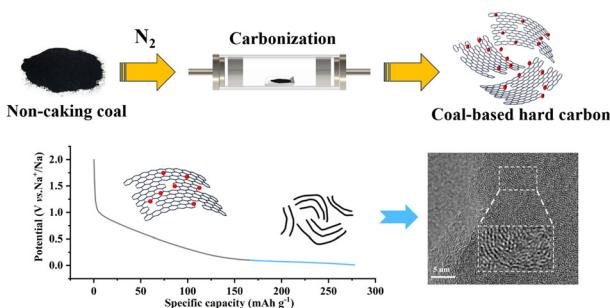
11737



## Insight into congener substitution effects on the combustion chemistry of tetramethoxysilane and tetramethoxymethane: an experimental and kinetic modeling study

Qilong Fang, Jun Fang, Tianyou Lian, Wei Li\* and Yuyang Li

11752



## Understanding the carbonization-controlled microstructure regulation in coal-based hard carbon to strengthen sodium storage performance

Yu Zhao, Ruyi Zhang, Jian Hao,\* Xiao Yang, Jianing Chen, Junli Guo\* and Caixia Chi

11762



## Substrate charge transfer drives the adsorption site of metal-phthalocyanines and porphyrins on coinage metal surfaces

Silvia Carlotto, Iulia Cojocariu, Vitaliy Feyer, Luca Schio, Luca Floreano and Maurizio Casarin\*

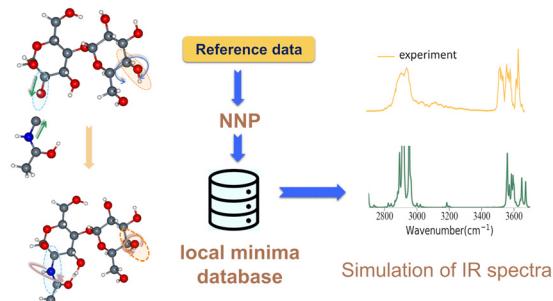


## RESEARCH PAPERS

11780

**Unraveling the low-energy conformers of neutral and charged mono- and di-saccharides with first-principles accuracy assisted by neural network potentials**

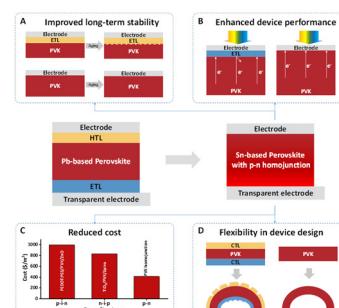
Huu Trong Phan, Pei-Kang Tsou, Hieu Cao Dong, Po-Jen Hsu and Jer-Lai Kuo\*



11792

**Numerical analysis of homojunction design for high-efficiency Pb-free perovskite solar cells**

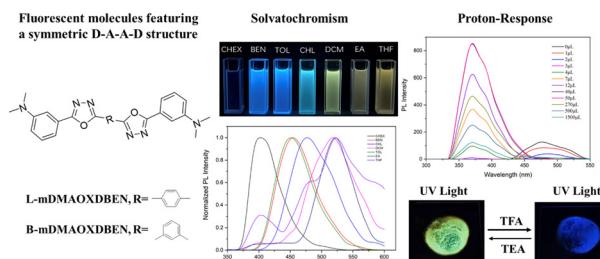
Bita Farhadi, Yufei Shao, Dan Yang, Kai Wang\* and Shengzhong Liu\*



11802

**Efficient fluorescence emission from protonated 1,3,4-oxadiazole derivatives with *meta*-dimethylamino substitution**

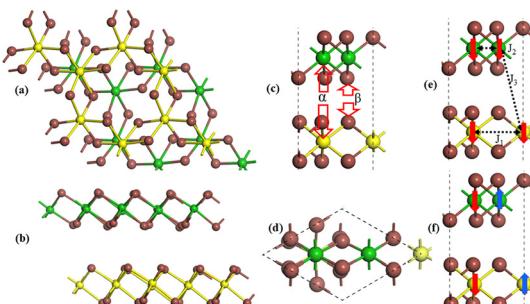
Yuhan Wang, Weitao Zheng, Binglian Bai, Jungang Cao,\* Jiarui Wu,\* Haitao Wang\* and Min Li\*



11811

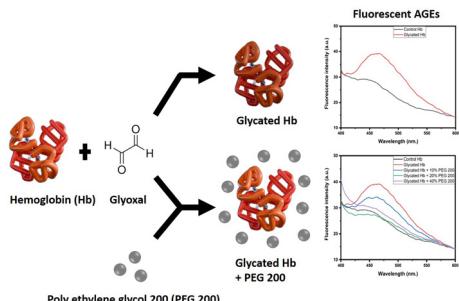
**Strain-dependent electronic, magnetic, and optical properties of a van der Waals  $\text{CrI}_3/\text{Vl}_3$  heterostructure: a first principles study**

Fazle Subhan, Luqman Ali, Nasir Shehzad, Yanguang Zhou,\* Zhenzhen Qin\* and Guangzhao Qin\*



## RESEARCH PAPERS

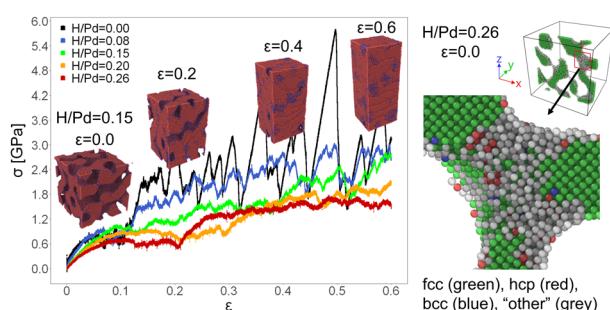
11821



### Understanding the impact of the molecular crowding environment on the glyoxal-mediated glycation of hemoglobin

Mangal Deep Burman, Sagar Bag, Souvik Ghosal and Sudipta Bhowmik\*

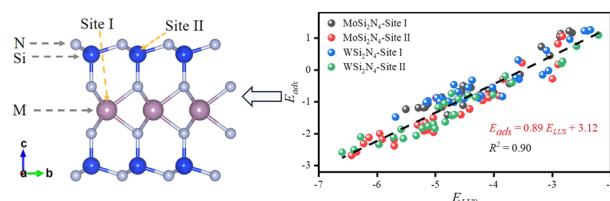
11830



### Mechanical behaviour of hydrogenated nanoporous palladium

Walter Schmidt,\* Thomas Castro, Eduardo Bringa, Max Ramírez, José Rogan and Felipe Valencia

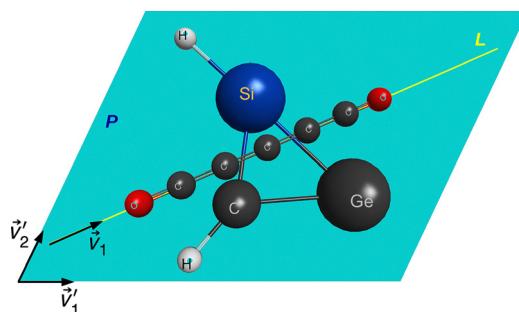
11842



### Activating lithium-ion storage performances of two-dimensional $MSi_2N_4$ ( $M = Mo, W$ ) monolayers: a theoretical prediction

Meng Tian

11853



### Tiling, propensity for planarity of the group-XIV pentatomic dihydrides $XYZH_2$ ( $X, Y, Z = C, Si, Ge$ ), and beyond

A. J. C. Varandas

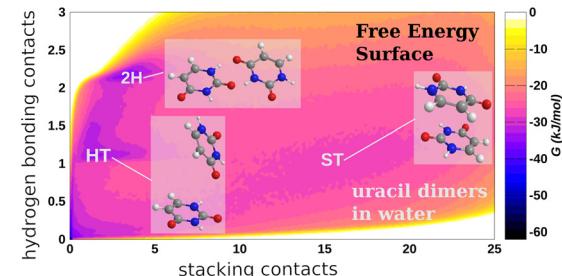


## RESEARCH PAPERS

11869

**Computational investigation of uracil dimers in water and the role of classical potentials**

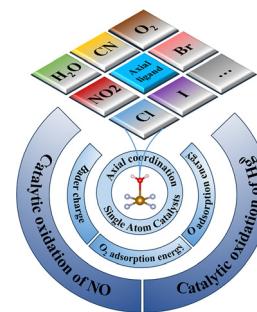
Tea Ostojić, Juraj Ovčar, Ali Hassanali and Luca Grisanti\*

**Well-tempered Metadynamics with Classical Force Fields**

11879

**Axial coordination engineering for single-atom catalysts in bifunctional oxidation of NO and mercury**

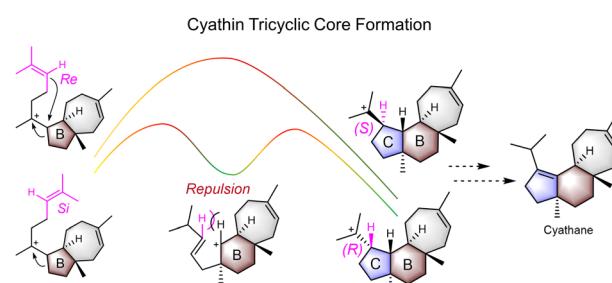
Jianghao Cai, Tongao Yao, Haoqi Tian, Xiaotian Tang, Yutong Jiang, Ruiyang Shi, Binghui Zhou, Zhengyang Gao and Weijie Yang\*



11887

**Probing intermediate folding patterns determined the carbon skeleton construction mechanism of cyathane diterpene**

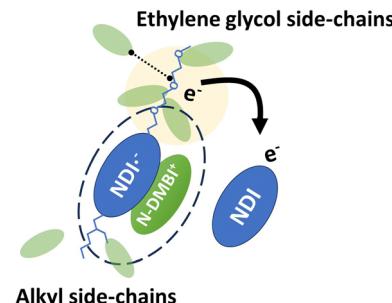
Kangwei Xu, Zhekai Xie, Xu Kang and Ruibo Wu\*



11898

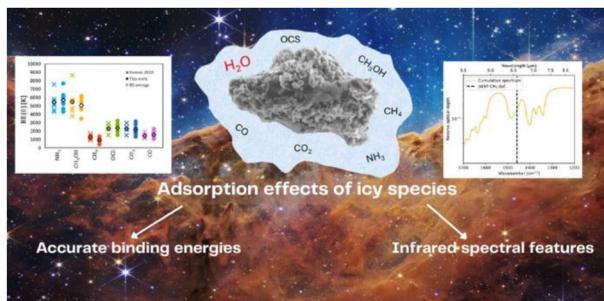
**Influence of imide side-chain functionality in the doping characteristics of naphthalenediimide derivatives as electron transport materials**

Wai Kin Yiu, Lewis Mackenzie, Dylan Wilkinson, Marcin Giza, Benjamin Vella, Michele Cariello, Stephen Sproules, Graeme Cooke\* and Pablo Docampo\*



## RESEARCH PAPERS

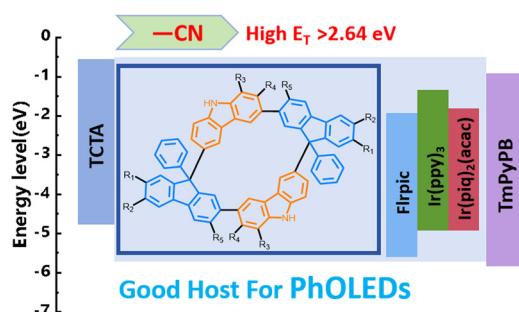
11907



**Predicting accurate binding energies and vibrational spectroscopic features of interstellar icy species. A quantum mechanical study**

Alicja Bulik, Berta Martínez-Bachs, Niccolò Bancone, Eric Mates-Torres, Marta Corno, Piero Ugliengo and Albert Rimola\*

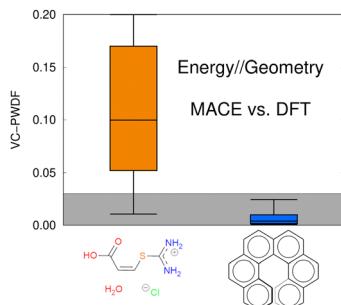
11920



**Theoretical studies of a novel carbazole–fluorene macrocycle as a host material for phosphorescent organic light-emitting diodes and the effects of substituents**

Zong-xiang Zheng, Wang-yang Wu, Hao-bo Wan, Wen-bin Xie, Jun Yang, Zhou Wang, Lei Yang,\* Xue-qin Ran\* and Ling-hai Xie\*

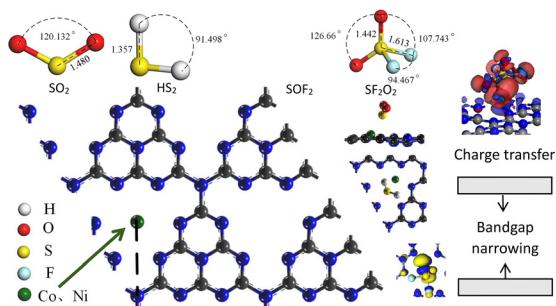
11930



**Assessment of a foundational machine-learned potential for energy ranking of molecular crystal polymorphs**

Cameron J. Nickerson and Erin R. Johnson\*

11941



**Study on the adsorption behavior, and electronic and gas-sensing properties of SF<sub>6</sub> decomposition products on Co- and Ni-modified g-C<sub>3</sub>N<sub>4</sub> monolayer films**

Zhiyuan Zhu, Qiuping Yang, Manyun Zhang and Jin Ye\*

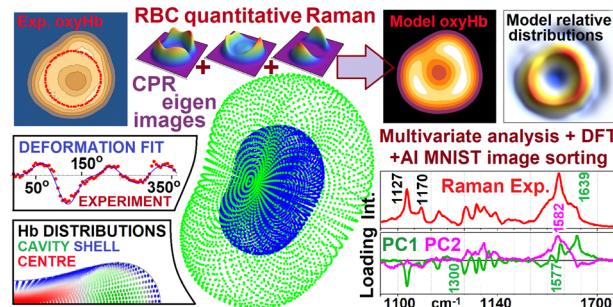


## RESEARCH PAPERS

11955

**Red blood cell Raman microscopy: modelling sub-cellular biochemistry**

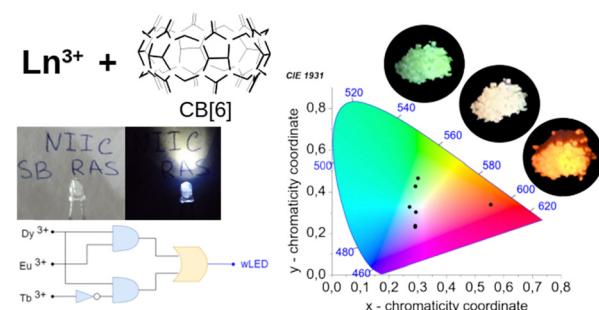
Victor V. Volkov, Joanna Aizenberg and Carole C. Perry\*



11974

**Multicolor luminescence of supramolecular compounds based on mixed Dy–lanthanide complexes and cucurbit[6]uril for logic gate operation and WLED application**

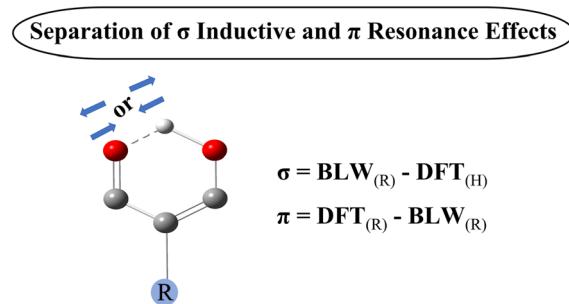
Mariana I. Rakhmanova, Taisiya S. Sukhikh, Irina V. Andrienko and Ekaterina A. Kovalenko\*



11986

**Separating  $\sigma$ -inductive and  $\pi$ -resonance effects of substituents on modulating resonance-assisted hydrogen bonds**

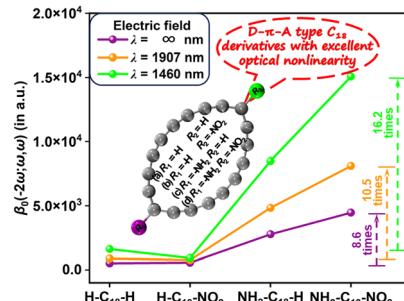
Xiaoli Lu, Shenghui Tang, Yan Zhang\* and Xuhui Lin\*



11993

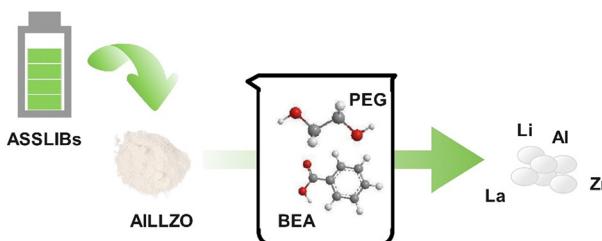
**Design of donor– $\pi$ –acceptor type cyclo[18]carbon derivatives for infrared nonlinear optical materials: a theoretical perspective**

Jingbo Xu, Jiaojiao Wang, Xiaohui Chen, Wenwen Zhao, Xiufen Yan, Zeyu Liu,\* Tian Lu\* and Aihua Yuan\*



## RESEARCH PAPERS

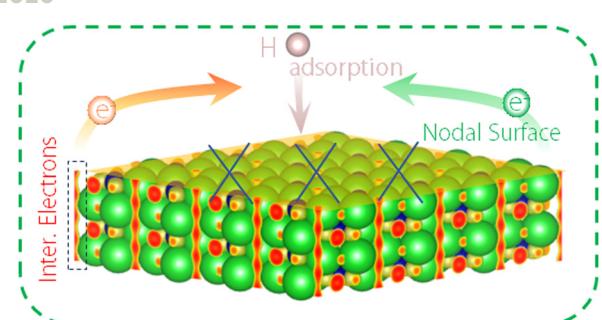
12004



**Green recovery of solid electrolytes from all-solid-state lithium-ion batteries using low-melting mixture solvents with tunable physical properties**

Yu Chen,\* Xueqing Zhang, Chenyang Wang, Zhuojia Shi, Xihou Wang, Jiayi Dong, Yanlong Wang and Minghui Feng

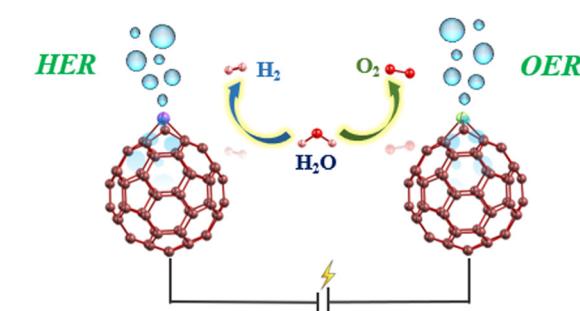
12016



**Cooperative adsorption performance of topological nodal surface fermions and excess electrons in a three-dimensional topological electride  $\text{Ba}_3\text{CrN}_3$**

Zhizuo Liu, Ying Liu,\* Zihan Li, Xuefang Dai, Xiaoming Zhang\* and Guodong Liu\*

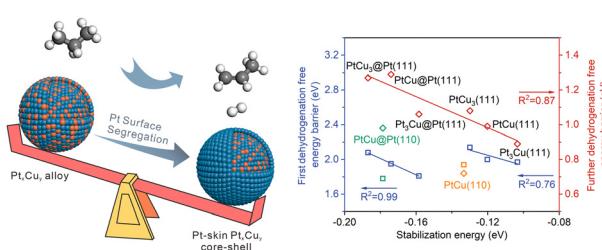
12024



**Metal-doped fullerene: promising electrocatalysts for hydrogen and oxygen evolution reactions**

Sougata Saha and Swapan K. Pati\*

12032



**Structural engineering of core–shell PtCu alloy catalysts for propane dehydrogenation: a DFT study**

Feifei Jiang, Shiyi Zhang, Daoru Liu, Jiajing Lin, Huayue Yang, Hexian Li, Haonan Wang, Guangxu Chen and Yun Zhao\*

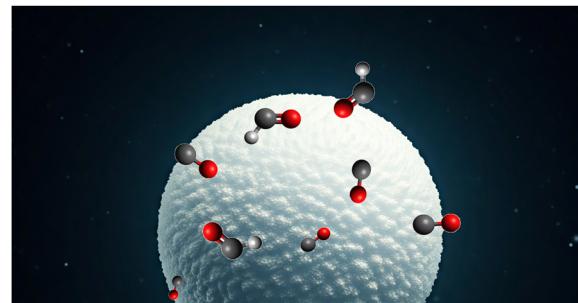


## RESEARCH PAPERS

12041

**First principles potentials for reactions on molecular crystals: modelling the interstellar H + CO reaction**

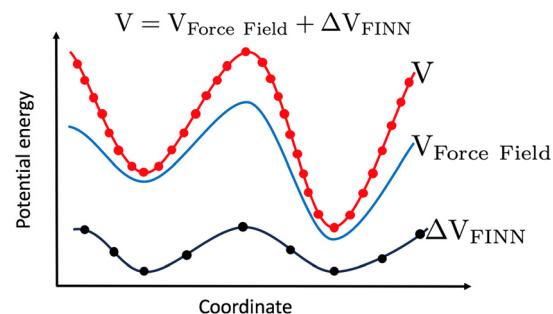
Terry J. Frankcombe



12051

**Fundamental invariant-neural network as a correction to the intramolecular force field illustrated for the full-dimensional potential energy surface of propane**

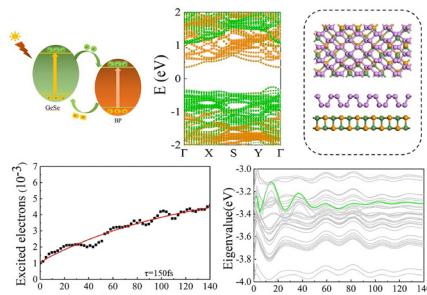
Liangfei Fu, Bina Fu\* and Dong H. Zhang\*



12060

**2D layered BP/group-IV monochalcogenide van der Waals heterostructures for photovoltaics: electronic structure, band alignment, and carrier dynamics**

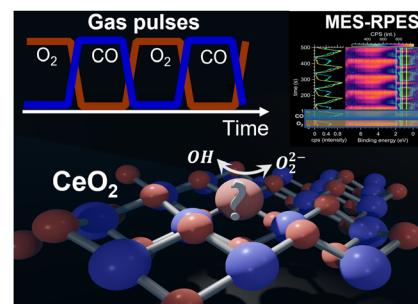
Kai Cheng,\* Peng Wu, Wenbo Hu, Guotai Zhang, Shijie Guo, Sandong Guo and Yan Su\*



12069

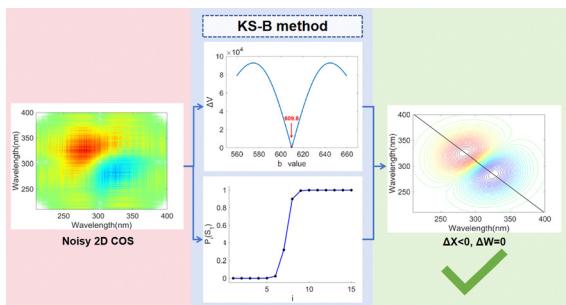
**Persistence of Ce<sup>3+</sup> species on the surface of ceria during redox cycling: a modulated chemical excitation investigation**

C. Hachemi, H. Dib, M. Debbichi, M. Badawi, C. Eads, M. Ibrahim, S. Loridant, J. Knudsen, H. Kaper and L. Cardenas\*



## RESEARCH PAPERS

12080

**A comprehensive statistical approach to identify correct types of cross-peaks based on their symmetric feature**

Linchen Xie, Anqi He, Limin Yang,\* Yukihiro Ozaki, Isao Noda, Yizhuang Xu\* and Kun Huang\*

## RETRACTION

12090

**Retraction: Impact of Ce doping on the optoelectronic and structural properties of a  $\text{CsPbI}_2$  perovskite solar cell**

M. I. Khan,\* Ali Mujtaba, Mahvish Fatima, Riadh Marzouki, Saddam Hussain and Tauseef Anwar

## CORRECTION

12091

**Correction: An investigation of contributors to the spin exchange interactions in organic pentacene–radical dyads using quasi-degenerate perturbation theory**

Philip S. Weiss, Amiel S. Paz and Claudia E. Avalos\*

