

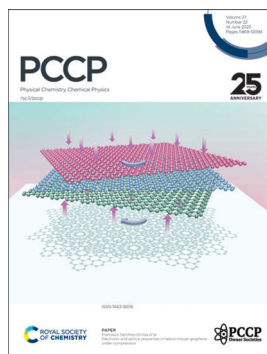
## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 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

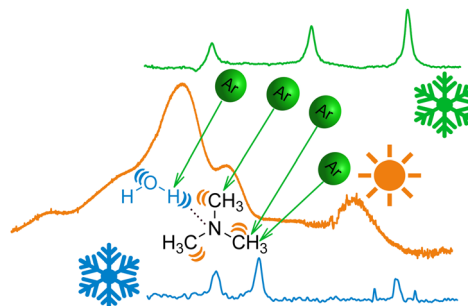
See Francisco Sánchez-Ochoa *et al.*, pp. 11541–11550. Image reproduced by permission of Francisco Sánchez-Ochoa from *Phys. Chem. Chem. Phys.*, 2025, 27, 11541.

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11487

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

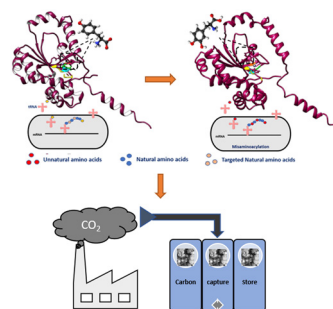
Taija L. Fischer, Casper V. Jensen, Eaindra Lwin, Dhritabrata Pal, Henrik G. Kjaergaard\* and Martin A. Suhm\*



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\*



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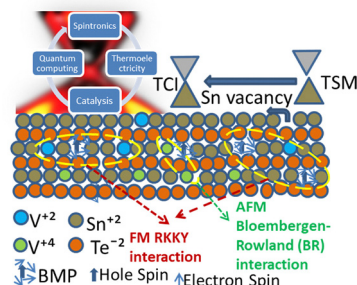
Fundamental questions  
Elemental answers

## RESEARCH PAPERS

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

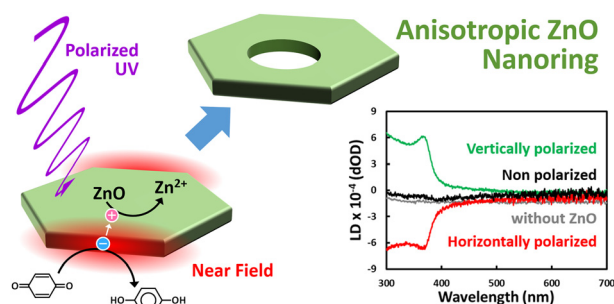
Subhadip Ghosh\* and Sanjeev Kumar Srivastava



11512

# Optically anisotropic ZnO nanorings fabricated using near-field photoelectrochemistry

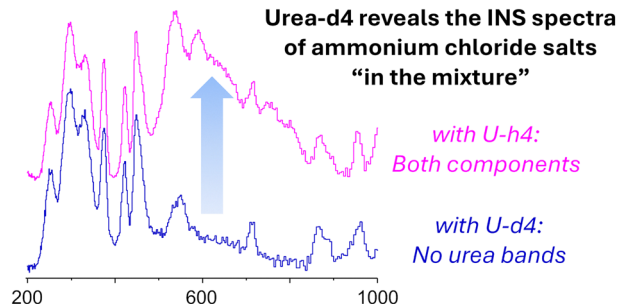
Yuki Oba, Seung Hyuk Lee and Tetsu Tatsuma\*



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

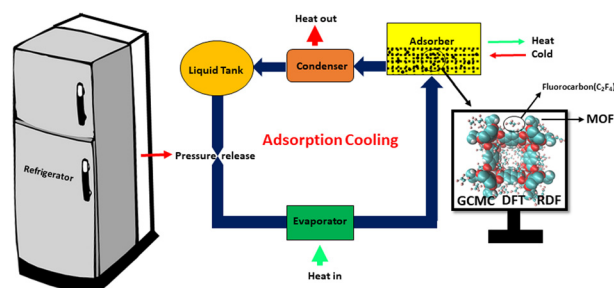
Rafael A. F. Serrano, Catarina F. Araújo, Paulo Ribeiro-Claro, Pedro D. Vaz, Svemir Rudić, João A. P. Coutinho and Mariela M. Nolasco\*



11530

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

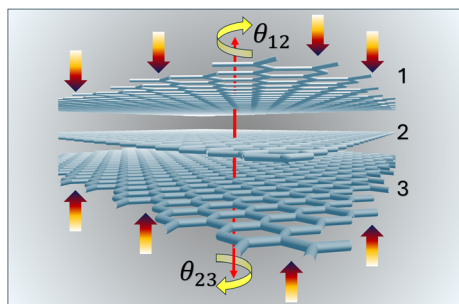
Dipankar Singha, Debansh Mohapatra and Malay Kumar Rana\*





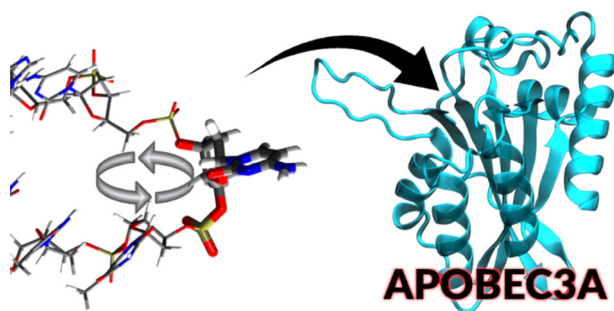
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11541

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

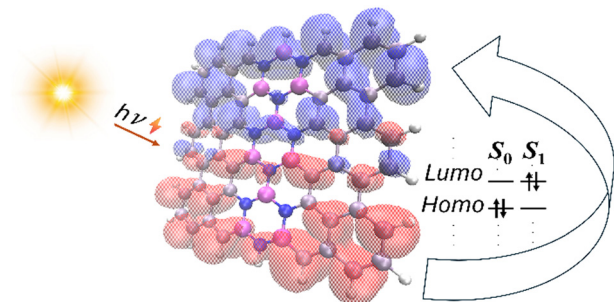
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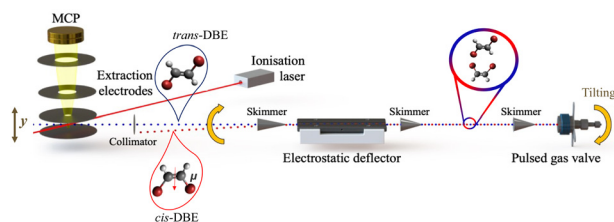
Mark A. Hix, A. G. Pramoda Sahankumari, Ashok S. Bhagwat and Alice R. Walker\*

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**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\*



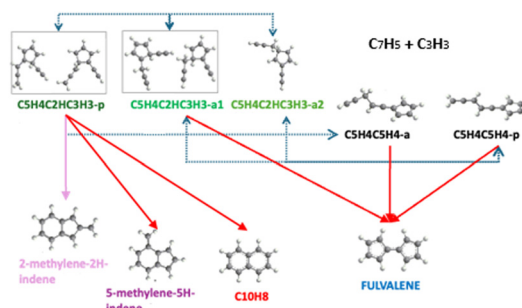


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# Rate constants of the fulvenallenyl recombination with propargyl and its role in PAH formation: a theoretical and kinetic modeling study

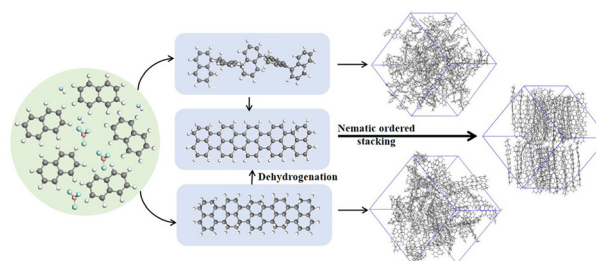
Alexander N. Morozov, Luna Pratali Maffei\* and Alexander M. Mebel\*



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

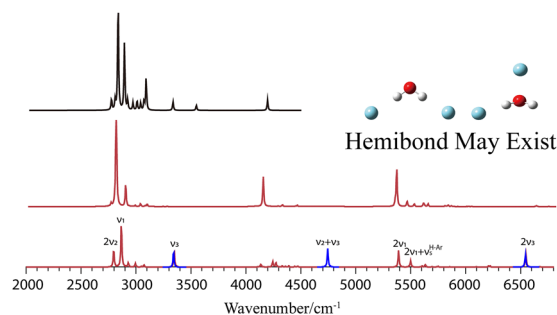
Xi Fan,\* Qiang Ren and Wen-kai Wei



11609

# Theoretical study on the structures and vibrational spectra of (H<sub>2</sub>O-Ar<sub>n</sub>)<sup>+</sup>, n = 1, 2: formation of a hemi-bond of water radical cation

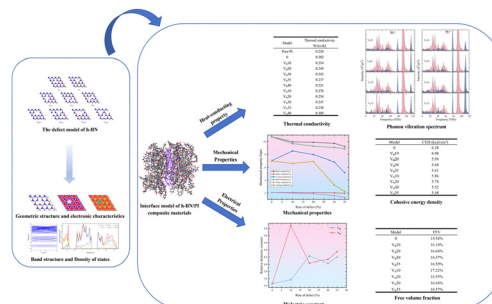
Jing-Min Liu,\* Qian-Rui Huang, Chih-Kai Lin and Jer-Lai Kuo\*



11617

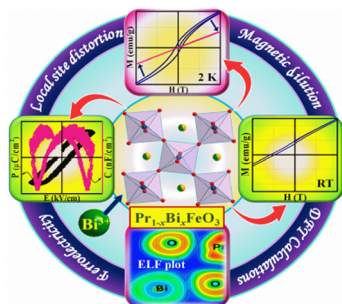
# Influence mechanism of vacancy defect effects on the intrinsic electronic properties of h-BN and the thermodynamic and dielectric properties of h-BN/PI interfaces

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



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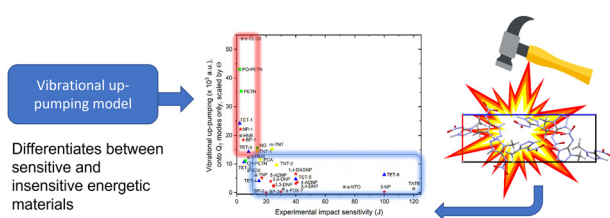
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### Implications of magnetic dilution of $\text{PrFeO}_3$ with $\text{Bi}^{3+}$ on its dielectric and magnetic properties

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

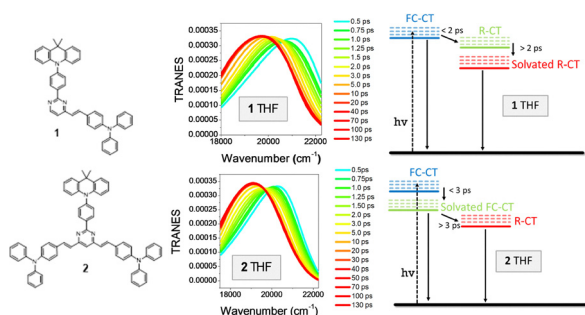
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### Predicting impact sensitivities for an extended set of energetic materials *via* the vibrational up-pumping model: molecular-based structure–property relationships identified

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

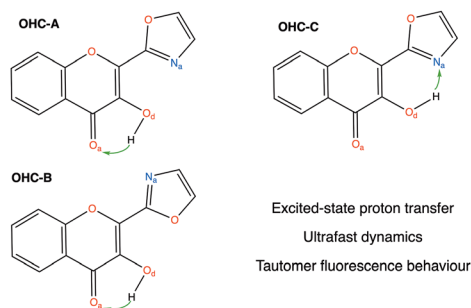
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### The role of branching in the ultrafast dynamics and two-photon absorption of two pyrimidine push–pull molecules

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

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

Dipangkali Sarma and Sai G. Ramesh\*

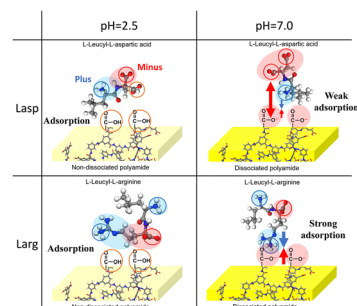


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# Molecular simulations and an experimental study of the oligopeptide-mediated fouling mechanisms of polyamide reverse-osmosis membranes

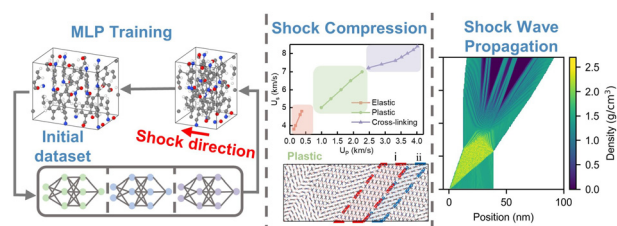
Ken Kinooka, Keizo Nakagawa, Hideto Matsuyama, Yu Fujimura, Takahiro Kawakatsu and Tomohisa Yoshioka\*



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

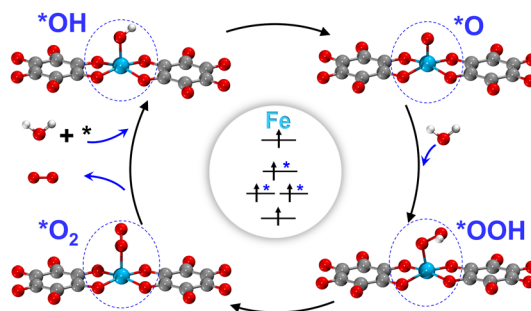
Lei Liu, Jingfu Shi, Di Song and Changqing Miao\*



11700

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

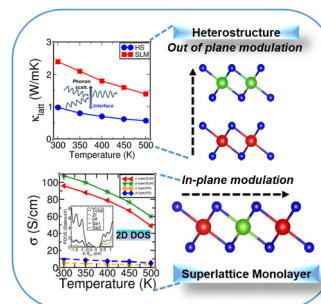
Erdembayalag Batsaikhan, Michitoshi Hayashi\* and Batjargal Sainbileg\*



11708

# Identifying key descriptors in ZrSe<sub>2</sub>/HfSe<sub>2</sub>-based heterostructures and superlattices for enhancing thermoelectric performance

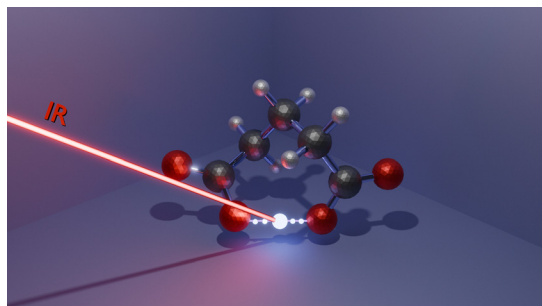
Tanu Choudhary, Satarupa Banik, Jipin Peter and Raju K. Biswas\*





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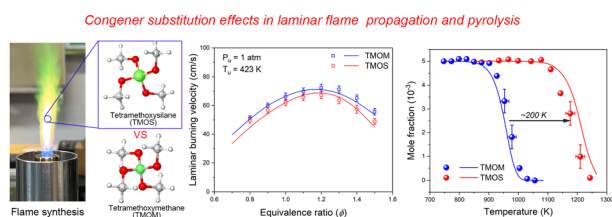
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### Intramolecular proton bonding in aliphatic dicarboxylate anions: dynamic conformational landscapes and spectral signatures

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

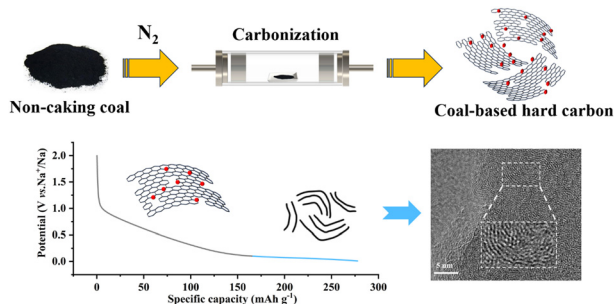
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### Insight into congener substitution effects on the combustion chemistry of tetramethoxysilane and tetramethoxymethane: an experimental and kinetic modeling study

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

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### 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

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### 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\*

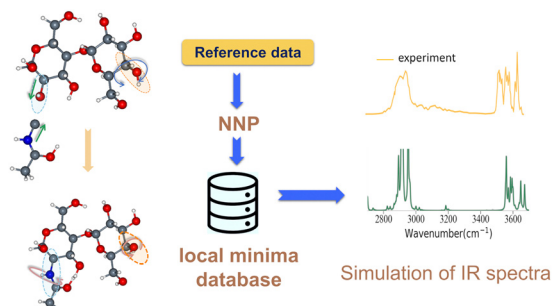


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# Unraveling the low-energy conformers of neutral and charged mono- and di-saccharides with first-principles accuracy assisted by neural network potentials

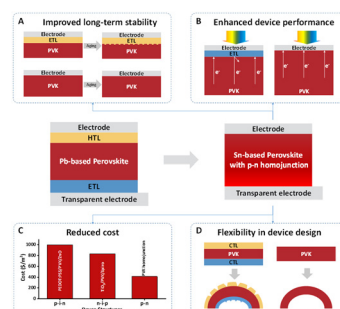
Huu Trong Phan, Pei-Kang Tsou, Hieu Cao Dong, Po-Jen Hsu and Jer-Lai Kuo\*



11792

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

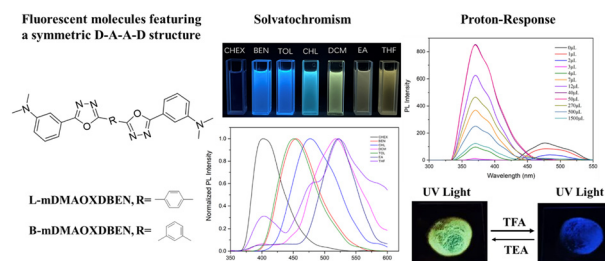
Bitu Farhadi, Yufei Shao, Dan Yang, Kai Wang\* and Shengzhong Liu\*



11802

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

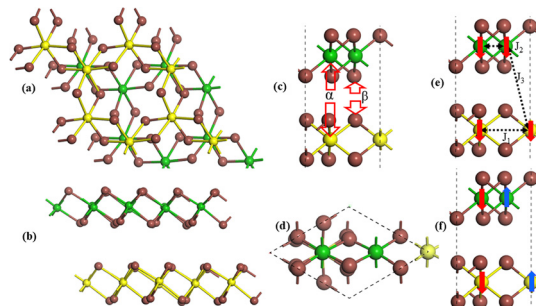
Yuhan Wang, Weitao Zheng, Binglian Bai, Jungang Cao,\* Jiarui Wu,\* Haitao Wang\* and Min Li\*



11811

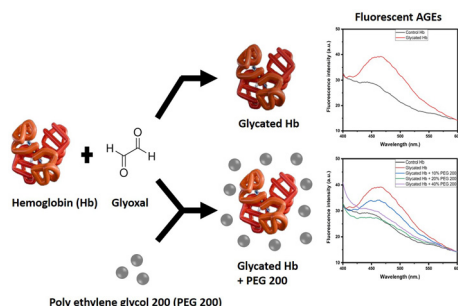
# Strain-dependent electronic, magnetic, and optical properties of a van der Waals CrI<sub>3</sub>/VI<sub>3</sub> heterostructure: a first principles study

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



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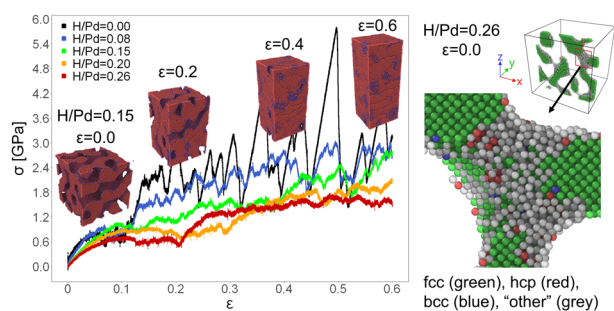
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### Understanding the impact of the molecular crowding environment on the glyoxal-mediated glycation of hemoglobin

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

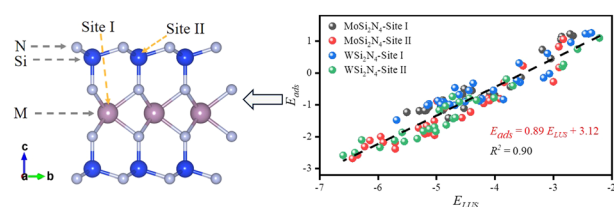
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### Mechanical behaviour of hydrogenated nanoporous palladium

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

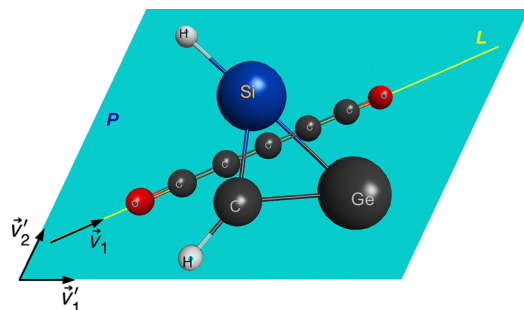
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### Activating lithium-ion storage performances of two-dimensional MSi<sub>2</sub>N<sub>4</sub> (M = Mo, W) monolayers: a theoretical prediction

Meng Tian

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### Tiling, propensity for planarity of the group-XIV pentatomic dihydrides XYZH<sub>2</sub> (X, Y, Z = C, Si, Ge), and beyond

A. J. C. Varandas

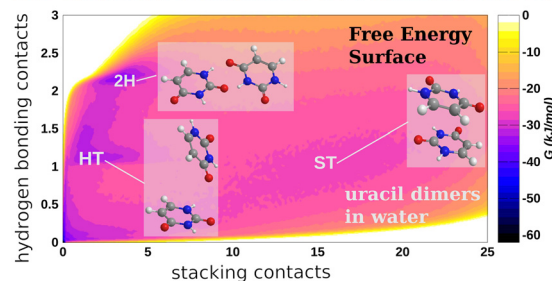


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**Computational investigation of uracil dimers in water and the role of classical potentials**

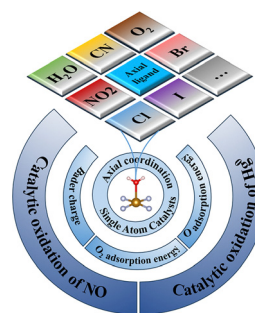
Tea Ostojić, Juraj Ovčar, Ali Hassanali and Luca Grisanti\*

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

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

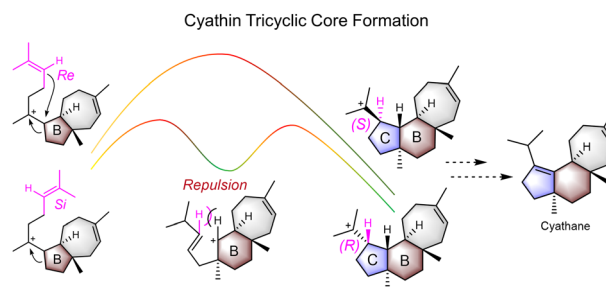
Jianghao Cai, Tongao Yao, Haoqi Tian, Xiaotian Tang, Yutong Jiang, Ruiyang Shi, Binghui Zhou, Zhengyang Gao and Weijie Yang\*



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

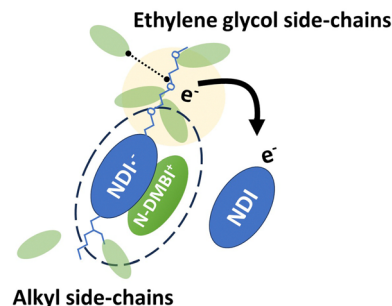
Kangwei Xu, Zhekai Xie, Xu Kang and Ruibo Wu\*



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

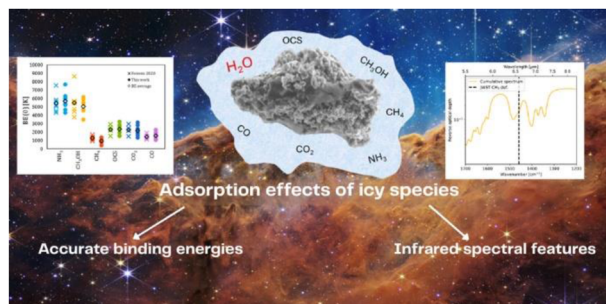
Wai Kin Yiu, Lewis Mackenzie, Dylan Wilkinson, Marcin Giza, Benjamin Vella, Michele Cariello, Stephen Sproules, Graeme Cooke\* and Pablo Docampo\*





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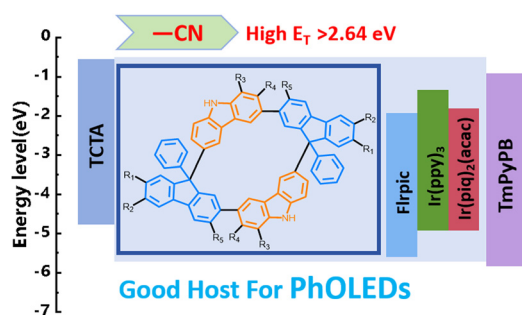
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### Predicting accurate binding energies and vibrational spectroscopic features of interstellar icy species. A quantum mechanical study

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

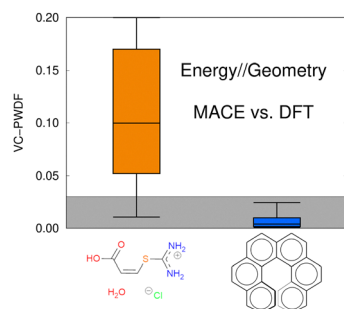
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### Theoretical studies of a novel carbazole-fluorene macrocycle as a host material for phosphorescent organic light-emitting diodes and the effects of substituents

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\*

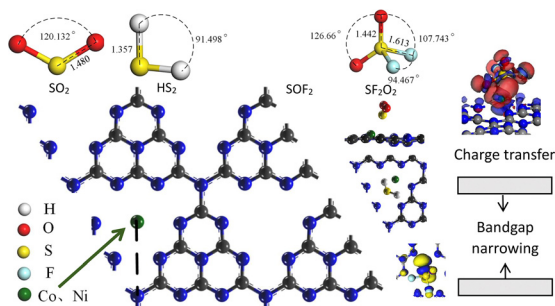
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### Assessment of a foundational machine-learned potential for energy ranking of molecular crystal polymorphs

Cameron J. Nickerson and Erin R. Johnson\*

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### 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\*

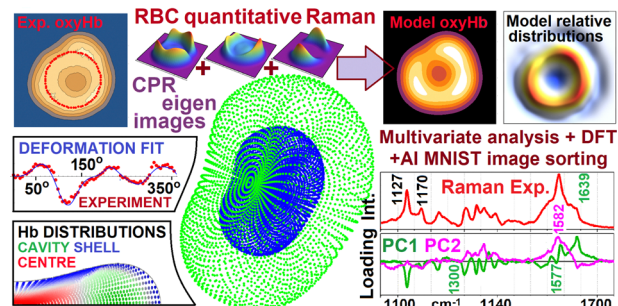


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## Red blood cell Raman microscopy: modelling sub-cellular biochemistry

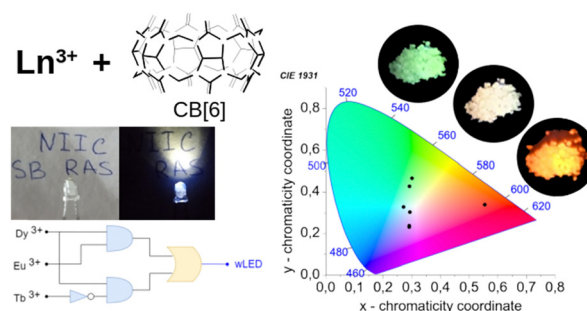
Victor V. Volkov, Joanna Aizenberg and Carole C. Perry\*



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

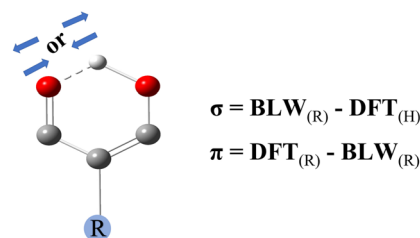
Mariana I. Rakhmanova, Taisiya S. Sukhikh, Irina V. Andrienko and Ekaterina A. Kovalenko\*



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

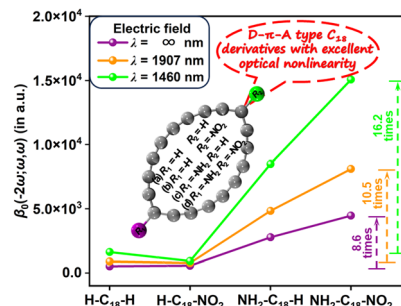
Xiaoli Lu, Shenghui Tang, Yan Zhang\* and Xuhui Lin\*

Separation of  $\sigma$  Inductive and  $\pi$  Resonance Effects

11993

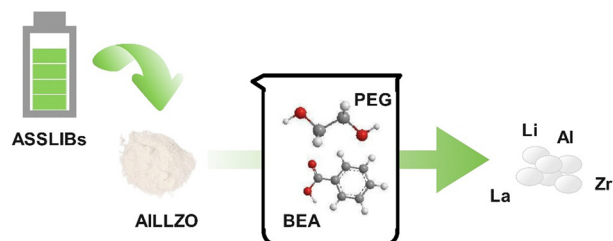
Design of donor– $\pi$ –acceptor type cyclo[18]carbon derivatives for infrared nonlinear optical materials: a theoretical perspective

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



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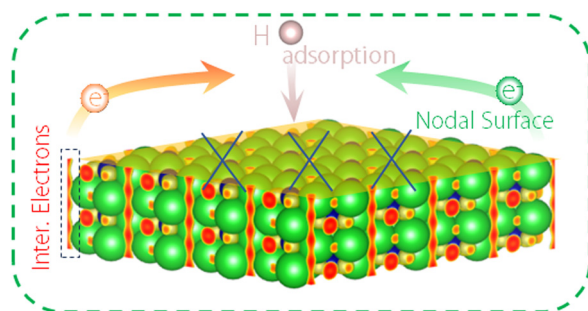
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### Green recovery of solid electrolytes from all-solid-state lithium-ion batteries using low-melting mixture solvents with tunable physical properties

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

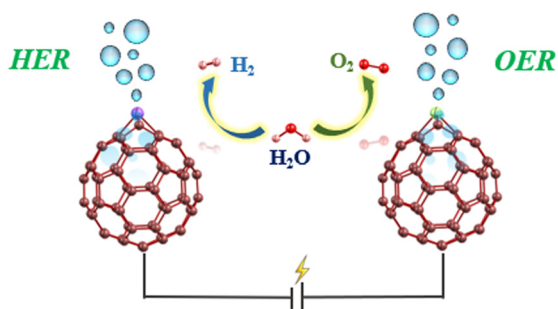
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### Cooperative adsorption performance of topological nodal surface fermions and excess electrons in a three-dimensional topological electride $\text{Ba}_3\text{CrN}_3$

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

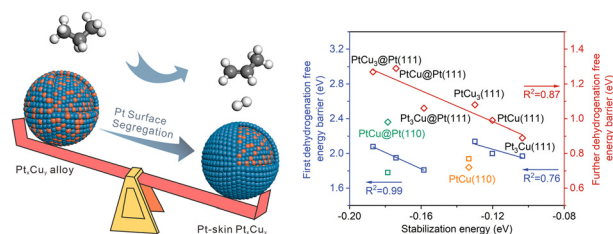
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### Metal-doped fullerene: promising electrocatalysts for hydrogen and oxygen evolution reactions

Sougata Saha and Swapan K. Pati\*

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### 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\*

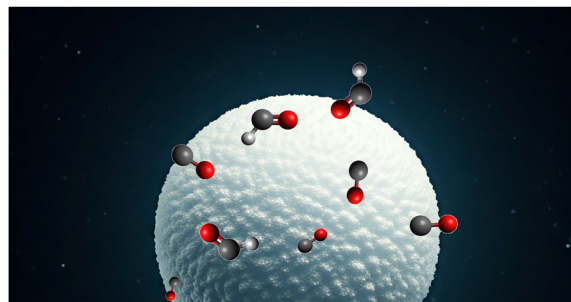


## RESEARCH PAPERS

12041

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

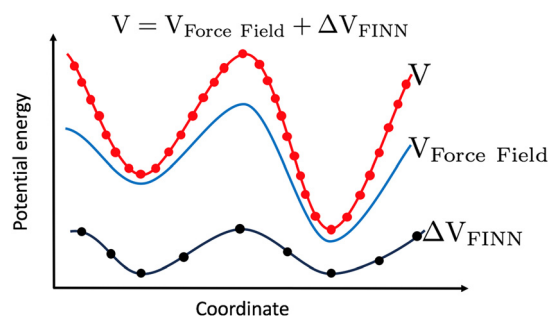
Terry J. Frankcombe



12051

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

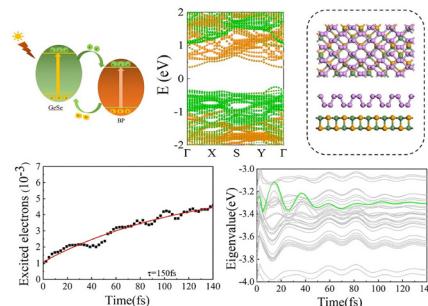
Liangfei Fu, Bina Fu\* and Dong H. Zhang\*



12060

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

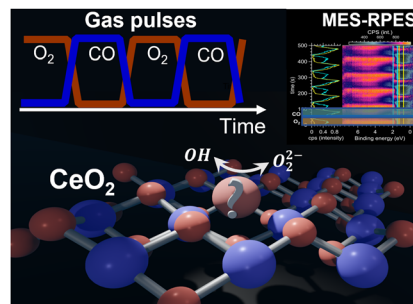
Kai Cheng,\* Peng Wu, Wenbo Hu, Guotai Zhang, Shijie Guo, Sandong Guo and Yan Su\*



12069

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

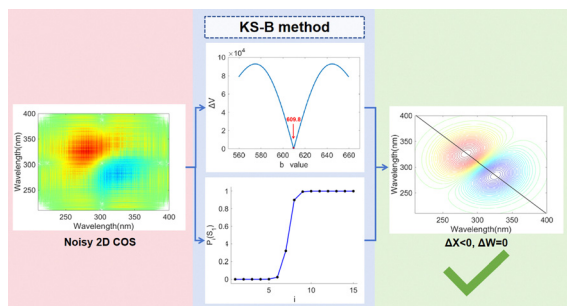
C. Hachemi, H. Dib, M. Debbichi, M. Badawi, C. Eads, M. Ibrahim, S. Loridant, J. Knudsen, H. Kaper and L. Cardenas\*





## 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 CsPbIBr<sub>2</sub> 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\*

