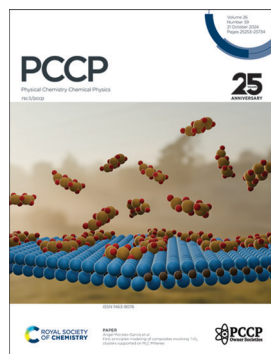


## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(39) 25253–25734 (2024)



### Cover

See Ángel Morales-García *et al.*, pp. 25319–25328. Image reproduced by permission of Ángel Morales-García from *Phys. Chem. Chem. Phys.*, 2024, 26, 25319.



### Inside cover

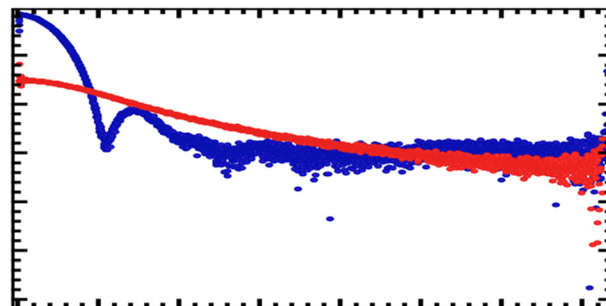
See Zhen Zhao, Bo Li *et al.*, pp. 25329–25340. Image reproduced by permission of Bo Li from *Phys. Chem. Chem. Phys.*, 2024, 26, 25329.

## REVIEWS

25268

### Perspectives on solution-based small angle X-ray scattering for protein and biological macromolecule structural biology

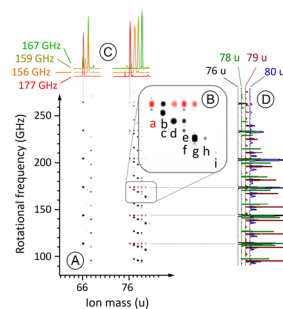
Ahmed S. A. Mohammed, Dmytro Soloviov and Cy M. Jeffries\*



25287

### Correlated rotational alignment spectroscopy: a new tool for high-resolution spectroscopy and the analysis of heterogeneous samples

Thomas Schultz



# Advance your career in science

with professional recognition that showcases  
your **experience, expertise and dedication**

## Stand out from the crowd

Prove your commitment  
to attaining excellence in  
your field

## Gain the recognition you deserve

Achieve a professional  
qualification that inspires  
confidence and trust

## Unlock your career potential

Apply for our professional  
registers (RSci, RSciTech)  
or chartered status  
(CChem, CSci, CEnv)

## Apply now

[rsc.li/professional-development](https://rsc.li/professional-development)

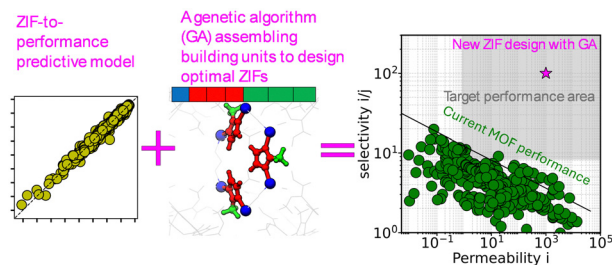


## COMMUNICATION

25314

## Inverse design of ZIFs through artificial intelligence methods

Panagiotis Krokidas,\* Michael Kainourgiakis, Theodore Steriotis and George Giannakopoulos

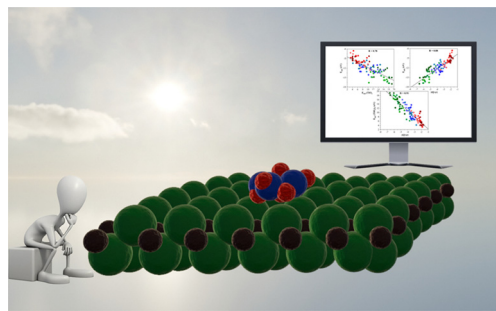


## RESEARCH PAPERS

25319

First principles modeling of composites involving TiO<sub>2</sub> clusters supported on M<sub>2</sub>C MXenes

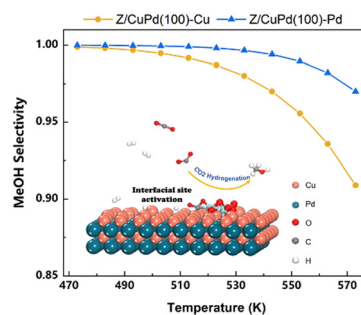
Masoomah Keyhanian, Néstor García-Romeral, Ángel Morales-García,\* Francesc Viñes and Francesc Illas



25329

Metal substrate engineering to modulate CO<sub>2</sub> hydrogenation to methanol on inverse Zr<sub>3</sub>O<sub>6</sub>/CuPd catalysts

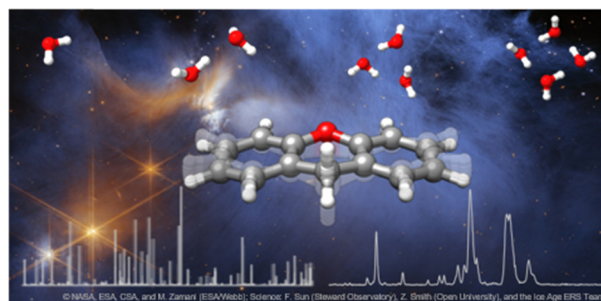
Bin Qin, XiaoYing Sun, Jianzhuo Lu, Zhen Zhao\* and Bo Li\*



25341

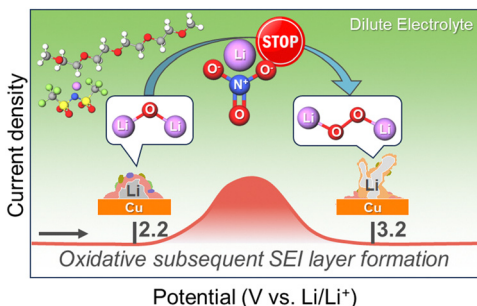
## Probing the structure and dynamics of the heterocyclic PAH xanthene and its water complexes with infrared and microwave spectroscopy

Donatella Loru,\* Wenhao Sun, Hugo Nootebos, Amanda L. Steber, Piero Ferrari and Melanie Schnell\*



## RESEARCH PAPERS

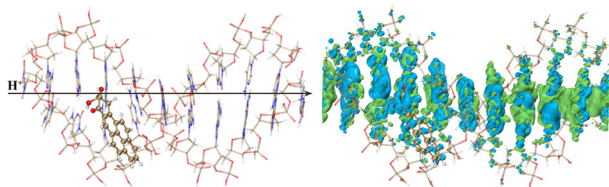
25352



### Revealing the enhancement of Li plating/stripping efficiency in TEGDME-based low-concentration electrolytes for anode-free lithium metal batteries

Yushen Wang and Hidenori Noguchi\*

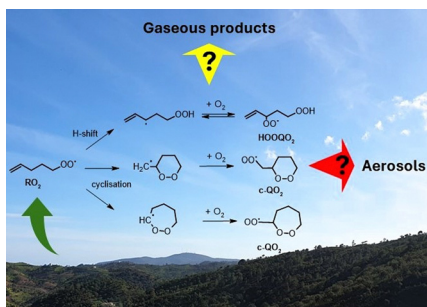
25363



### Effects of BPQ binding on the nonadiabatic dynamics of excited electrons in poly(dG)–poly(dC) DNA under proton irradiation

Zihua Hu, Zun-Yi Deng and Hong-Jian Feng\*

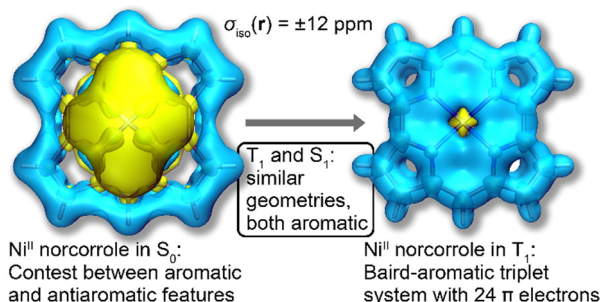
25373



### H-shift and cyclization reactions in unsaturated alkylperoxy radicals near room temperature: propagating or terminating autoxidation?

Barbara Nozière\* and Luc Vereecken\*

25385



### Excited-state aromaticity reversals in norcorrole

Peter B. Karadakov\* and Edward Cummings

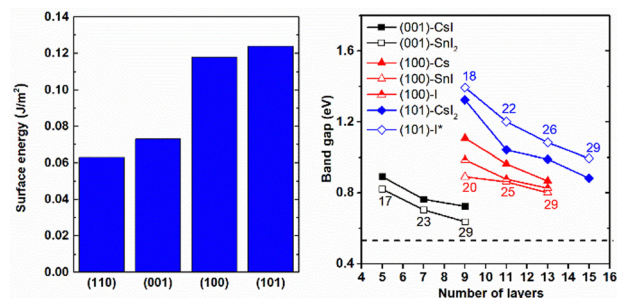


## RESEARCH PAPERS

25393

### First-principles study of the surface energies and electronic structures of $\gamma$ -CsSnI<sub>3</sub> surfaces

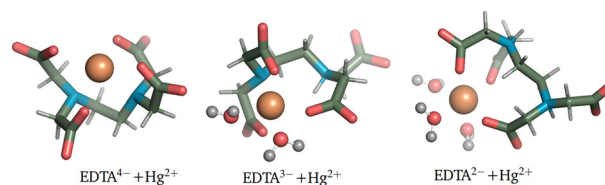
Tong Zhou, Yan-Jin Chen, Chunju Hou\* and Yi Yang\*



25402

### Role of EDTA protonation in chelation-based removal of mercury ions from water

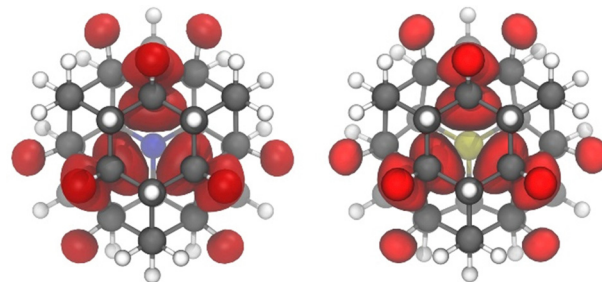
Halyna Butovych,\* Fatemeh Keshavarz, Bernardo Barbiellini, Erkki Lähderanta, Jaroslav Ilnytskyi and Taras Patsahan\*



25412

### Heteroatom-vacancy centres in molecular nanodiamonds: a computational study of organic molecules possessing triplet ground states through $\sigma$ -overlap

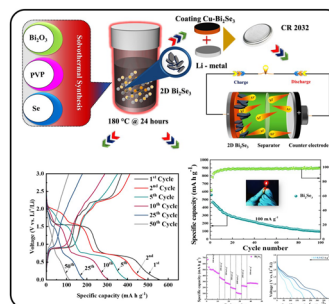
Colette Maya Macarios, Jiří Pittner, Viki Kumar Prasad and Ulrich Fekl\*



25418

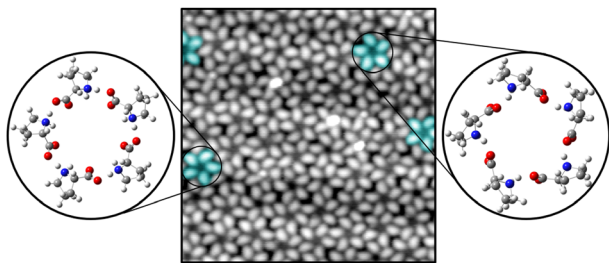
### Exploring the electrochemical performance of layered Bi<sub>2</sub>Se<sub>3</sub> hexagonal platelets as the anode material for lithium-ion batteries

Shaik M. Abzal, Sumit Khatua, Kurapati Kalyan, SaiLakshmi Janga, Rajkumar Patel,\* L. N. Patro\* and Jatis Kumar Dash\*



## RESEARCH PAPERS

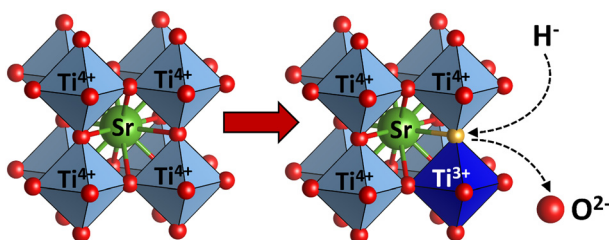
25430



### Enantiopure molecules form apparently racemic monolayers of chiral cyclic pentamers

Benjamin R. Heiner, Kaitlyn M. Handy, Angela M. Devlin, Jewel L. Soucek, Alexander M. Pittsford, David A. Turner, Jacob P. Petersen, Allen G. Oliver, Steven A. Corcelli and S. Alex Kandel\*

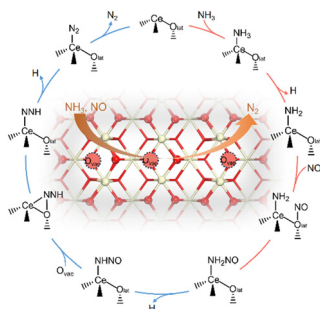
25439



### The spectroscopy of hydride in single crystals of SrTiO<sub>3</sub> perovskite

William R. Palfey,\* Son-Jong Hwang, William A. Goddard III and George R. Rossman

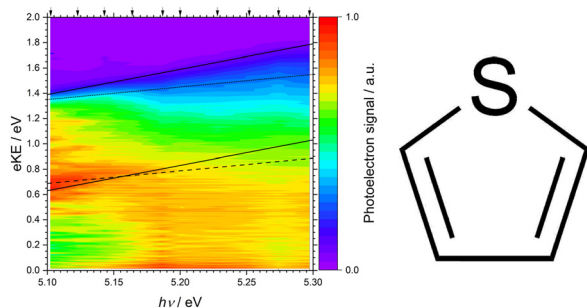
25452



### Mechanistic insights into NH<sub>3</sub>-assisted selective reduction of NO on CeO<sub>2</sub>: a first-principles microkinetic study on selectivity and activity

Danfeng Xiong, Yang Chen, Haiyang Yuan\* and Haifeng Wang

25461



### A multiphoton ionisation photoelectron imaging study of thiophene

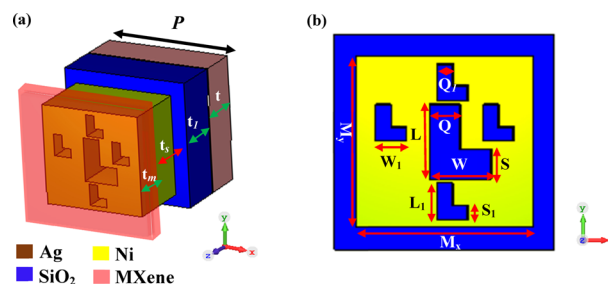
Joseph J. Broughton, Sarbani Patra, Michael A. Parkes, Graham A. Worth and Helen H. Fielding\*



25469

### A high-performance ultra-wideband metasurface absorber and thermal emitter for solar energy harvesting and thermal applications

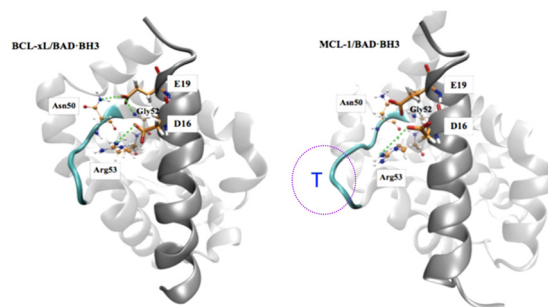
Ammar Armghan, Meshari Alsharari, Muhammad Abuzar Baqir, Muhammad Saqlain\* and Khaled Aliqab



25480

### Theoretical study on the selective binding of BH3-only protein BAD to anti-apoptotic protein BCL-xL instead of MCL-1

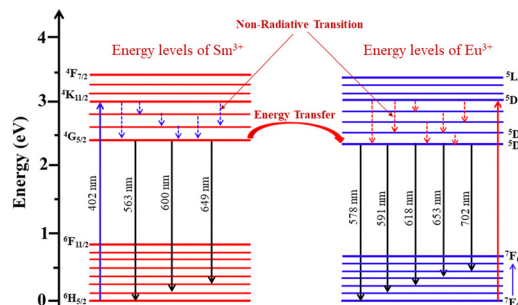
Panpan Wang, Jinglan Cui,\* Guojie Cheng and Dawei Zhang\*



25488

### Eu<sup>3+</sup> singly-doped and Eu<sup>3+</sup>/Sm<sup>3+</sup> co-doped ZnS quantum dots: structure, optical properties and energy transfer

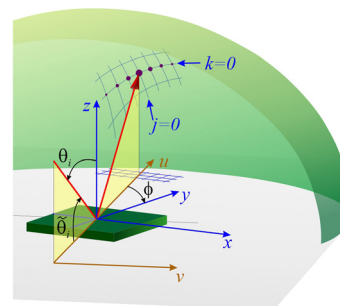
N. T. M. Thuy, T. T. T. Huong, N. T. Hien, N. T. Luyen, N. T. Kien, N. T. K. Van, P. M. Tan, N. D. Vinh, T. Ngoc and N. X. Ca\*



25501

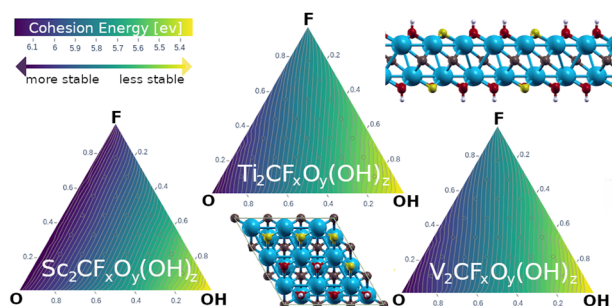
### Grazing incidence fast atom diffraction: general considerations, semiclassical perturbation theory and experimental implications

E. Pollak, P. Roncin, W. Allison and S. Miret-Artés\*



## RESEARCH PAPERS

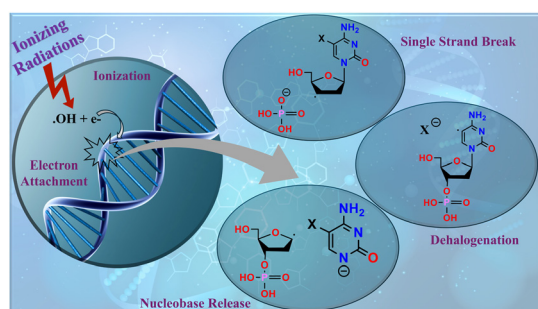
25514



## The effect of mixed termination composition in Sc, Ti, and V-based MXenes

Michal Novotný, Karolína Tkáčová and František Karlický\*

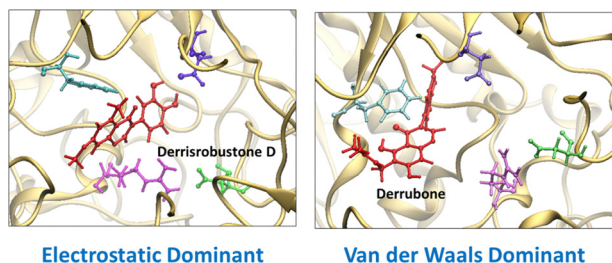
25524



## Dissociative electron attachment to halogenated nucleotides: a quest for better radiosensitizers

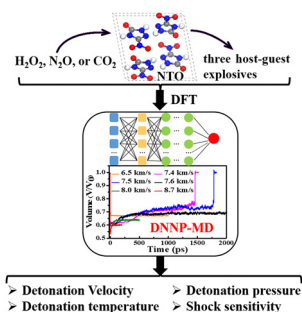
Shubham Kumar and Manabendra Sarma\*

25533

The potentiality of isoflavones from *Derris robusta* (DC.) Benth. against  $\alpha$ -glucosidase

Pakuna Panbo, Cholpisut Tantapakul and Apirak Payaka\*

25543



## Detonation performance and shock sensitivity of energetic material NTO with embedded small molecules: a deep neural network potential accelerated molecular dynamics study

Caimu Wang, Jidong Zhang, Wei Guo,\* Ruibin Liu and Yugui Yao

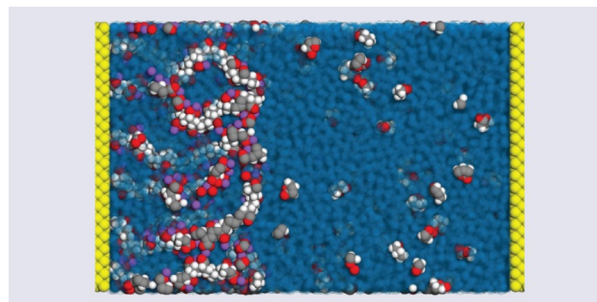


## RESEARCH PAPERS

25557

### All-atom molecular dynamics simulations showing the dynamics of small organic molecules in water-solvated polyelectrolyte brush layers

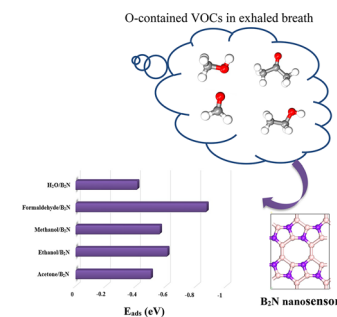
Leon A. Smook,\* Raashiq Ishraaq, Tanmay Sarkar Akash, Sissi de Beer and Siddhartha Das



25567

### Exploring the adsorption behavior of O-containing VOCs in human breath on a B<sub>2</sub>N monolayer using DFT simulations

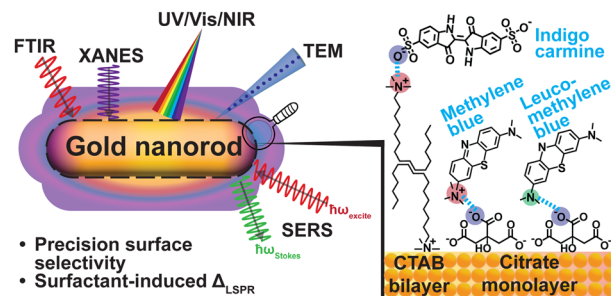
Rezvan Rahimi\* and Mohammad Solimannejad\*



25581

### Targeted synthesis of gold nanorods and characterization of their tailored surface properties using optical and X-ray spectroscopy

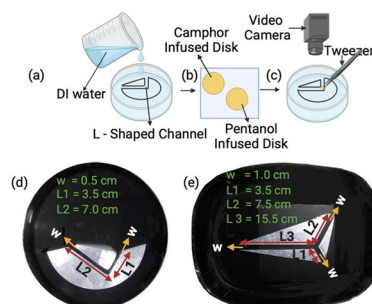
David G. Schauer, Jona Bredehoeft, Umar Yunusa, Ajith Pattammattel, Hans Jakob Wörner and Emily A. Sprague-Klein\*



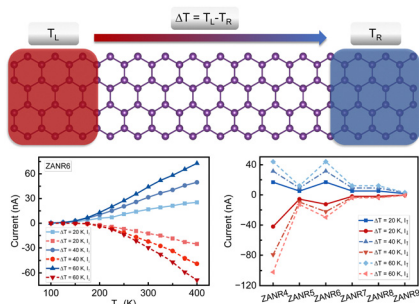
25590

### Surface tension gradient invoked path selection

Anjuman Ara Khatun,\* Aarsh Chotalia, Kalpita Das, Shiva Dixit and P. Parmananda



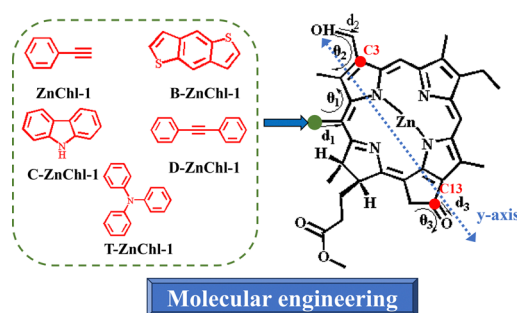
25599



### Spin-dependent Seebeck effect in zigzag-edge antimonene nanoribbons

Liyan Lin, Yue Jiang,\* Xinyi Gao, Yandong Guo,\* Hongli Zeng and Xiaohong Yan\*

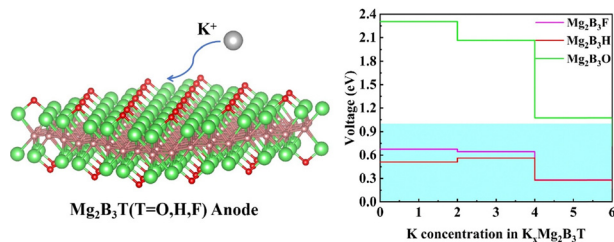
25607



### Molecular engineering and structure–property relationship based on D–A chlorophyll derivative and the application in organic solar cells

Kaiyan Zhang, Ting Li, Peng Song,\* Fengcai Ma and Yuanzuo Li\*

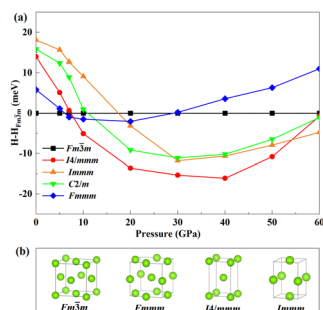
25623



### Two-dimensional functionalized MBene $Mg_2B_3T$ ( $T = O, H,$ and $F$ ) monolayers as anode materials for high-performance K-ion batteries

Fengzhang Tang,\* Jiafei Pang,\* Jinni Yang, Xiaoyu Kuang\* and Aijie Mao\*

25632



### Structural evolution and superconductivity of thorium under high pressure and its modulation

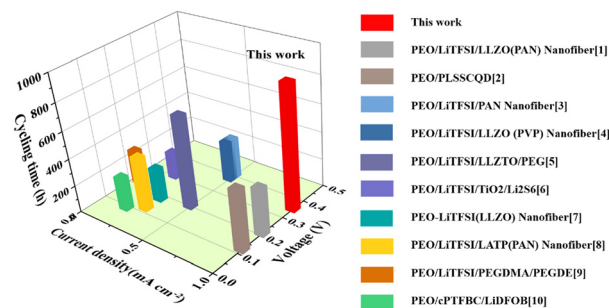
Lihui Zhan, Wenhao Fan, Junyi Miao, Shi He, Qingzhuo Duan, Xilong Dou and Cheng Lu\*



25640

### A strategy involving the use of 3D self-supporting B-N co-doped carbon nanofiber composite solid polymer electrolytes to stabilize the interface between polymer electrolytes and lithium metal

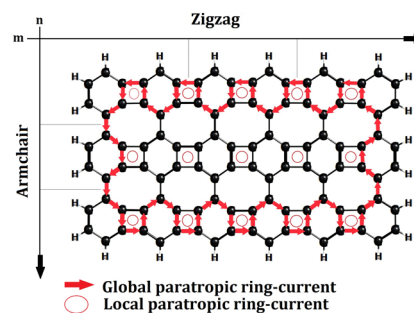
Yujie Wang,\* Lingling Sun, Xiaoli Li and Yan Zhang



25648

### Aromaticity of biphenylene networks

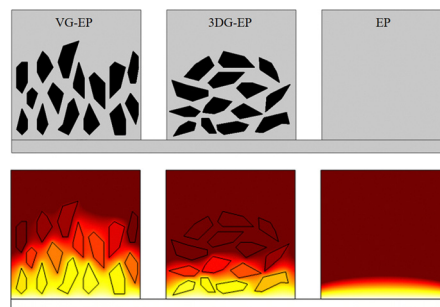
Lenara I. Valiulina,\* R. Valiyev, Victor N. Cherepanov and Elena V. Stepanova



25655

### Enhancing thermal transport of epoxy composites with vertically aligned graphene *in situ* grown on the thermal interface

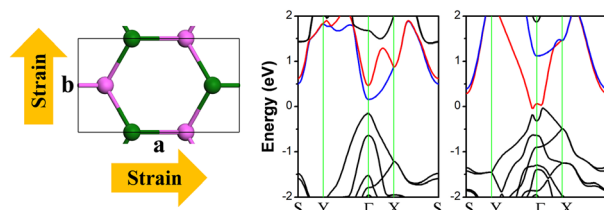
Jiaqiang Liao, Shijie Chen, Minjin Huang, Tao Rui, Zhi Qun Tian and Changzheng Li\*



25664

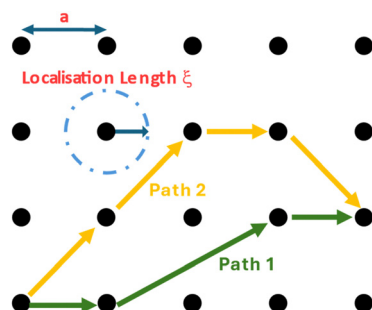
### Strain-tunable electronic anisotropy of the AlSb double-layer honeycomb structure

Hongsheng Liu,\* Yaning Li, Rui Chen, Yuanyuan Zhao and Junfeng Gao\*



## RESEARCH PAPERS

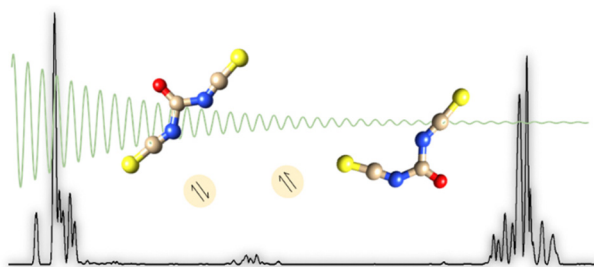
25670



### Theoretical analysis of electron transport in perovskite thin films

Ankur Bhaumik\* and Anshu Pandey

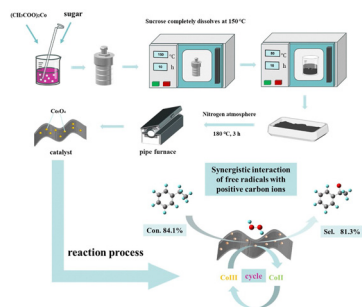
25678



### Rotational conformers and nuclear spin isomers of carbonyl diisothiocyanate

Eva Gougoula,\* Jonathan Pfeiffer, Melanie Schnell\* and Frank Tambornino\*

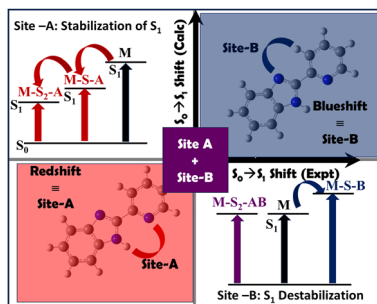
25688



### Green and efficient catalytic oxidation of ethylbenzene to acetophenone over cobalt oxide supported on a carbon material derived from sugar

Jinhong Li, Zhimei Song, Kaikai Cui, Haonan Li, Mei Han, Jing Wang and Lidong Chen\*

25697



### Spectroscopic characterization of the complexes of 2-(2'-pyridyl)-benzimidazole and (H<sub>2</sub>O)<sub>1,2</sub>, (CH<sub>3</sub>OH)<sub>1,2</sub>, and (NH<sub>3</sub>)<sub>1,2</sub> isolated in the gas phase

Arkaprabha Sen, Saurabh Khodia, Ramesh Jarupula, Simran Baweja, Bhavika Kalal and Surajit Maity\*

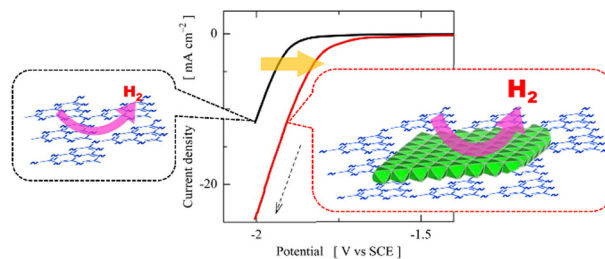


## RESEARCH PAPERS

25709

### Enhanced electrocatalytic activity in hydrogen evolution reaction using 2D/2D nanohybrids of ruthenate nanoflakes and graphitic carbon nitride

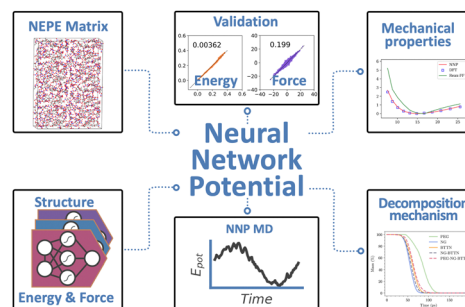
Takayuki Ban,\* Kazuki Inukai, Chika Takai-Yamashita and Kazuhiro Manseki



25719

### Uncovering the decomposition mechanism of nitrate ester plasticized polyether (NEPE): a neural network potential simulation

Mingjie Wen, Juntao Shi, Xiaoya Chang, Jiahe Han, Kehui Pang, Dongping Chen and Qingzhao Chu\*



## CORRECTION

25731

### Correction: Effects of BPQ binding on the nonadiabatic dynamics of excited electrons in poly(dG)–poly(dC) DNA under proton irradiation

Zhijia Hu, Zun-Yi Deng and Hong-Jian Feng\*

