

# PCCP

Physical Chemistry Chemical Physics – An international journal

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## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(9) 4499–4978 (2025)



### Cover

See Ralph A. Wheeler and Emily E. Dalbey, pp. 4593–4602. Image reproduced by permission of Ralph A. Wheeler from *Phys. Chem. Chem. Phys.*, 2025, 27, 4593. Image generated with AI



### Inside cover

See Zhiyong Xu and Jian Zhou, pp. 4603–4613. Image reproduced by permission of Jian Zhou from *Phys. Chem. Chem. Phys.*, 2025, 27, 4603.

## PROFILE

4514

**Physical Chemistry Chemical Physics profiles: contributors to the 2024 Emerging Investigators collection**

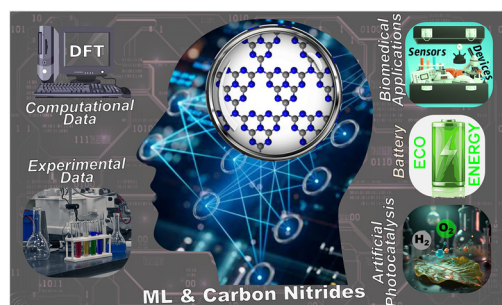


## REVIEWS

4531

**Navigating the evolution of two-dimensional carbon nitride research: integrating machine learning into conventional approaches**

Deep Mondal, Sujoy Datta\* and Debnarayan Jana\*



# RSC Applied Polymers

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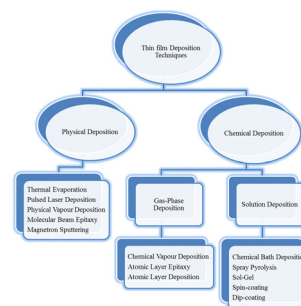
Fundamental questions  
Elemental answers

## REVIEWS

4567

## Review on the optical and electrical properties of chalcogenide thin films: challenges and applications

W. A. Abd El-Ghany

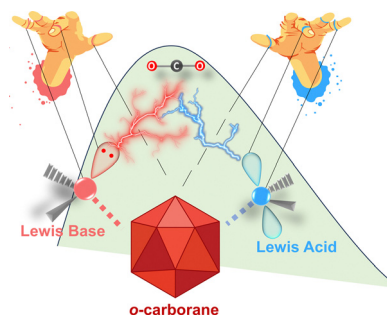


## COMMUNICATION

4587

Puppeteering the reactivity of frustrated Lewis pairs toward CO<sub>2</sub> via coordination dichotomy in bridging units

Mohammad Faizan and Ravinder Pawar\*

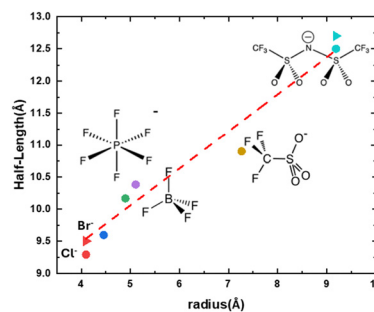


## RESEARCH PAPERS

4593

## Structure factor line shape model gives approximate nanoscale size of polar aggregates in pyrrolidinium-based ionic liquids

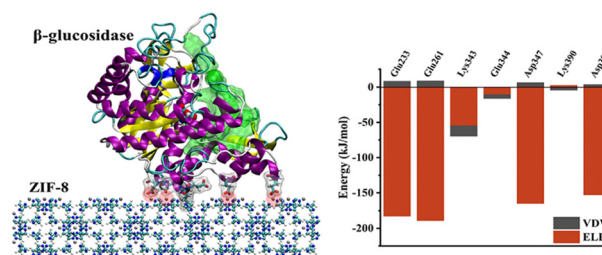
Ralph A. Wheeler\* and Emily E. Dalbey



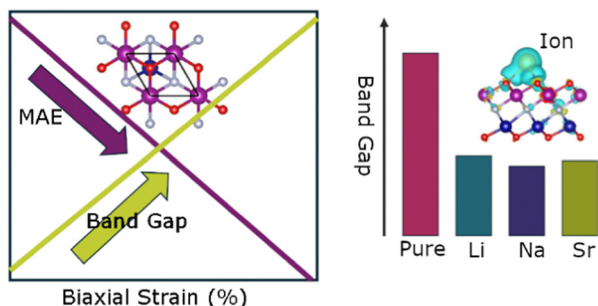
4603

## Unraveling the orientation of an enzyme adsorbed onto a metal–organic framework

Zhiyong Xu and Jian Zhou\*



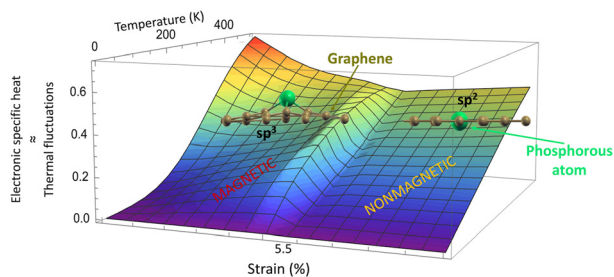
4614



### Modulation of the electronic and magnetic properties of an $\text{MnCrNO}_2$ ferromagnetic semiconductor MXene

Sudil Sandeepa Dewamuni, Buddi Oshada Vithanage, Deniz Çakır and Edirisuriya M. Dilanga Siriwardane\*

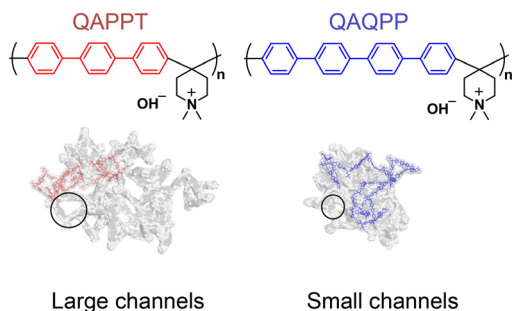
4627



### Magnetic quantum phase transition extension in strained P-doped graphene

Natalia Cortés,\* J. Hernández-Tecorralco, L. Meza-Montes, R. de Coss and Patricio Vargas

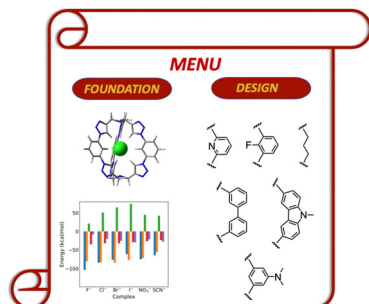
4634



### Atomic insights into the ion-conducting channels of poly(arylene piperidinium) anion exchange membranes

Weiwen Pu and Zhaoru Sun\*

4643



### Computer-aided design of triazolo-cages as anion receptors

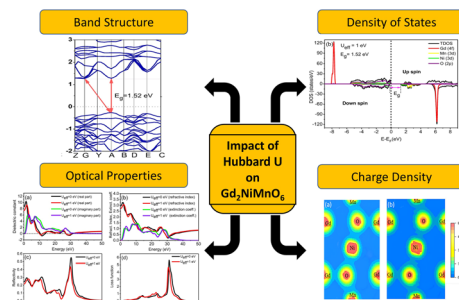
Minwei Che, Sibali Debnath, Amar H. Flood and Krishnan Raghavachari\*



4652

### An *ab initio* approach to investigate the impact of Hubbard $U$ correction on the physical properties of $\text{Gd}_2\text{NiMnO}_6$ double perovskite

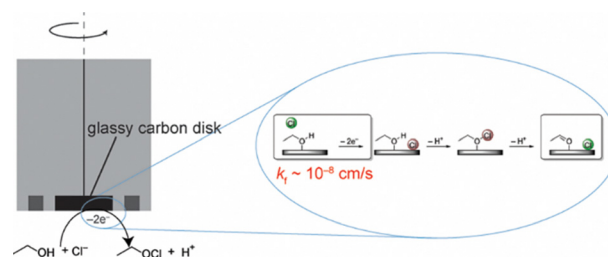
Md. Yasir Arafat, Sweetly Akter, Md. Ferdous Shanto, M. J. Hosen\* and M. D. I. Bhuyan\*



4663

### Insights into the mechanism of electrochemical chloride oxidation in ethanol from X-ray photoelectron spectroscopy, quiescent solution voltammetry, and rotating ring-disk electrodes

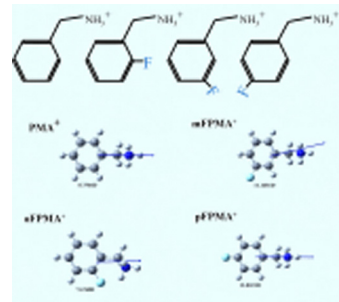
Ryan D. Van Daele, Siqi Li, Katherine H. Morrissey and Bart M. Bartlett\*



4669

### Preparation of high-performance quasi-two-dimensional (Q-2D) perovskite solar cells by fluorinated benzylamine groups at different substitution positions

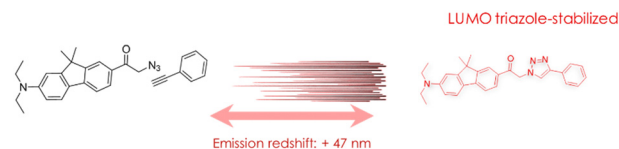
Longtao Du, Jianhua Liao, Kegui Li, Yuge Chang, Qiang Huang, Xiaoyan Gan,\* Liling Guo and Hanxing Liu



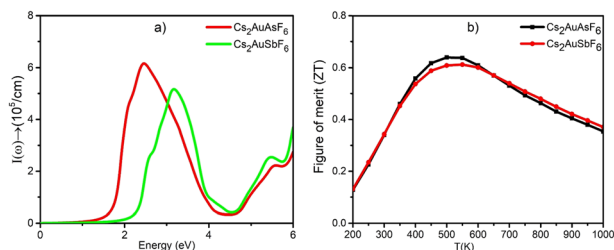
4679

### Click and shift: the effect of triazole on solvatochromic dyes

Jean Rouillon,\* Carlos Benitez-Martin, Morten Grøtli and Joakim Andréasson\*



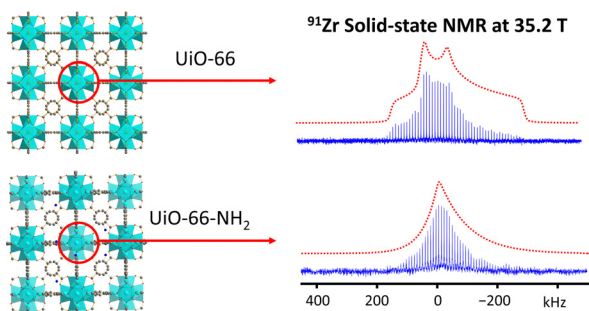
4686



### Novel $\text{Cs}_2\text{Au}^{\text{I}}\text{M}^{\text{III}}\text{F}_6$ ( $\text{M} = \text{As}, \text{Sb}$ ) double halide perovskites: sunlight and industrial waste heat management device applications

Shuaib Mahmud,\* Usama Ahmed,  
Md. Atik Uz Zaman Atik, Md. Mukter Hossain,  
Md. Mohi Uddin and Md. Ashraf Ali\*

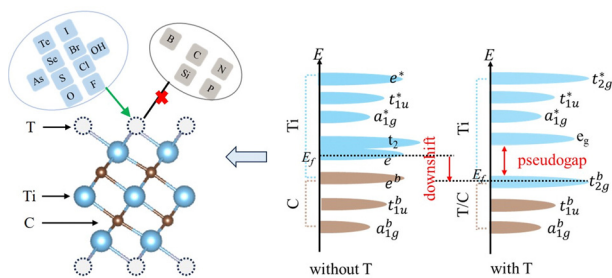
4704



### Local order, disorder, and everything in between: using $^{91}\text{Zr}$ solid-state NMR spectroscopy to probe zirconium-based metal–organic frameworks

Wanli Zhang, Bryan E. G. Lucier, Vinicius Martins,  
Tahereh Azizivahed, Ivan Hung, Yijue Xu, Zhehong Gan,  
Amrit Venkatesh, Tian Wei Goh, Wenyu Huang,  
Aaron J. Rossini and Yining Huang\*

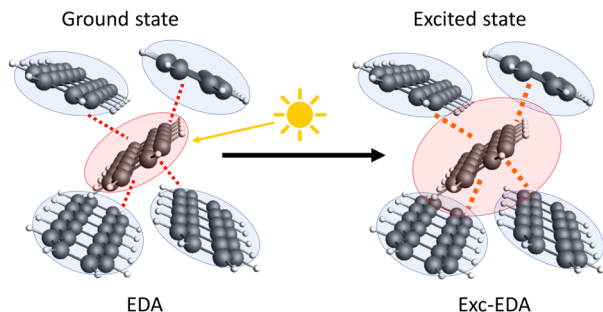
4717



### Rational design of surface termination of $\text{Ti}_3\text{C}_2\text{T}_2$ MXenes for lithium-ion battery anodes

Meng Tian

4728



### Energy decomposition analysis for excited states: an extension based on TDDFT

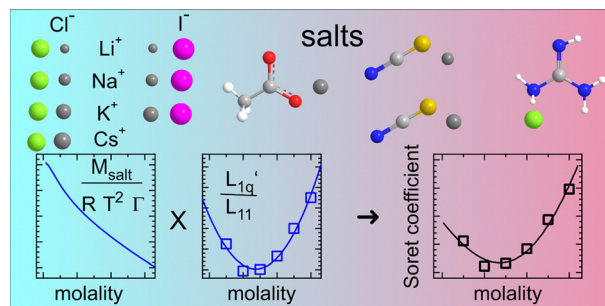
Florian Kreuter and Ralf Tonner-Zech\*



4746

### Analyzing the concentration-dependent Soret coefficient minimum in salt solutions: an overview

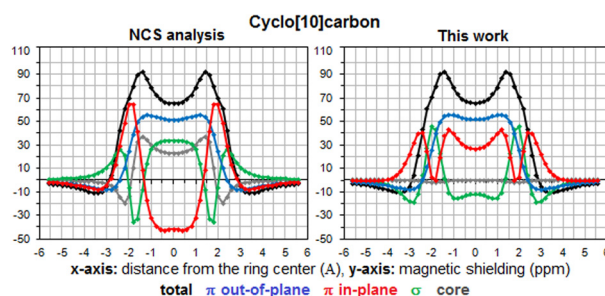
Binny A. Rudani, W. J. Briels\* and Simone Wiegand\*



4756

### Orbital contributions to the magnetic shielding of cyclo[2n]carbons ( $n = 3-12$ )

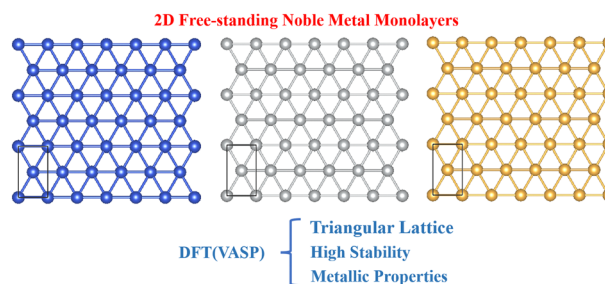
Marija Baranac-Stojanović



4766

### Structure, stability and electronic properties of two-dimensional monolayer noble metals with triangular lattices: Cu, Ag, and Au

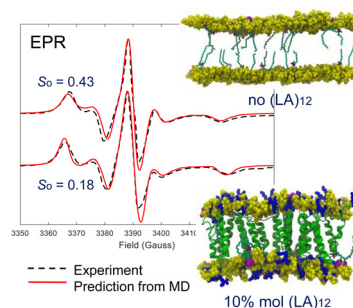
Zhefeng Wang, Kai Chen, Youmin Xu, Zengjie Wang, Lingbao Kong, Songyou Wang\* and Wan-Sheng Su\*



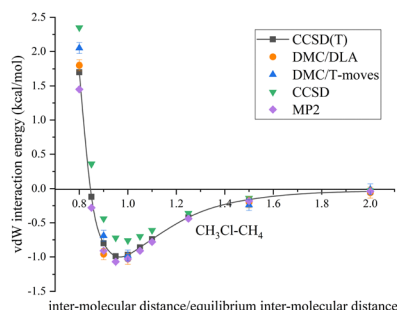
4775

### Predicting and interpreting EPR spectra of POPC lipid bilayers with transmembrane $\alpha$ -helical peptides from all-atom molecular dynamics simulations

Andrea Catte and Vasily S. Oganessian\*



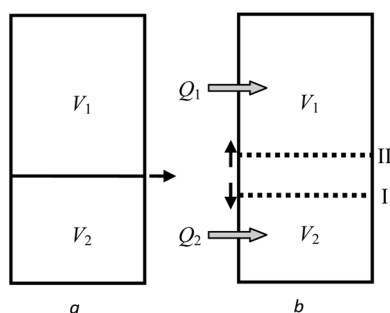
4785



### Accuracy of the diffusion quantum Monte Carlo method on dissociation curves of van der Waals systems with the single-Slater–Jastrow trial wavefunction

Zhiru Huang, Xiaojun Zhou and Fan Wang\*

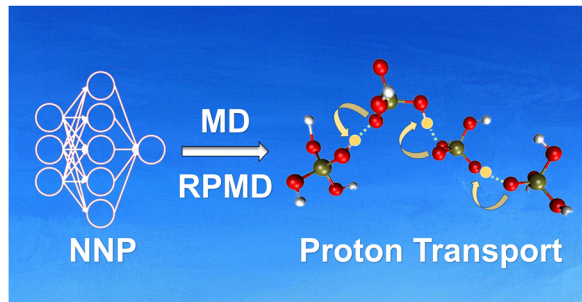
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### Mixing of real and quantum gases

Andrey Ya. Borshchevskii\*

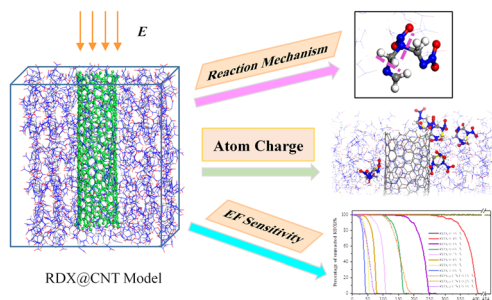
4804



### Proton transport in liquid phosphoric acid: the role of nuclear quantum effects revealed by neural network potential

Pei Liu, Wei Li\* and Shuhua Li\*

4814



### Reaction mechanism and sensitivity enhancement of energetic materials doped with carbon nanotubes under electric fields by molecular dynamics simulations

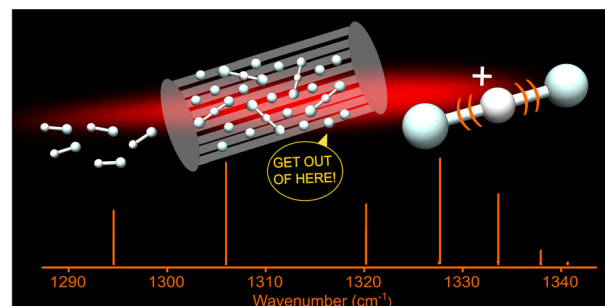
Junjian Li, Junying Wu,\* Yiping Shang, Yule Yao, Ruizheng Liu, Jianyu Wang and Lang Chen



4826

High-resolution leak-out spectroscopy of  $\text{HHe}_2^+$ 

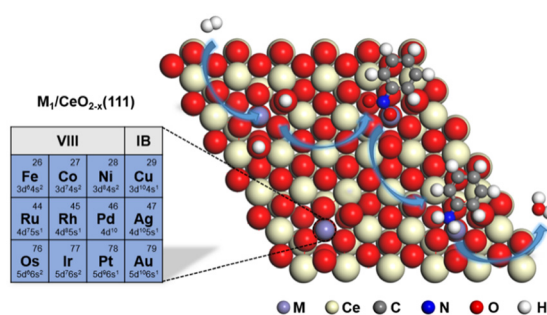
Thomas Salomon, Carlo Baddeliyanage, Carla Schladt, Irén Simkó, Attila G. Császár, Wesley G. D. P. Silva, Stephan Schlemmer and Oskar Asvany\*



4829

Theoretical study on nitrobenzene hydrogenation to aniline catalyzed by  $\text{M}_1/\text{CeO}_{2-x}$  (111) single-atom catalysts

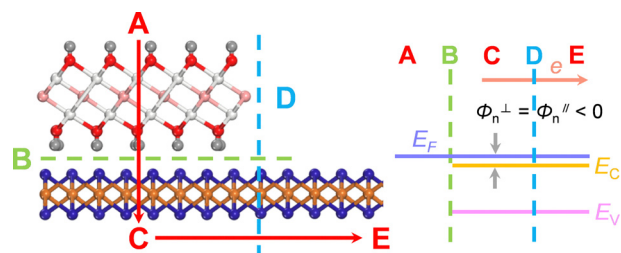
Haohao Wang, Min Pu and Ming Lei\*



4837

Functionalized  $\text{Sc}_2\text{N}$  as Ohmic-contact electrodes for monolayer  $\text{PtSe}_2$ : an *ab initio* study

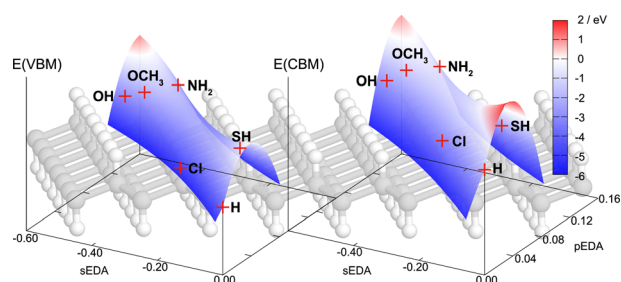
Hong Li,\* Jiahui Li, Chaoyang Fan, Fengbin Liu, Shuai Sun and Jing Lu\*



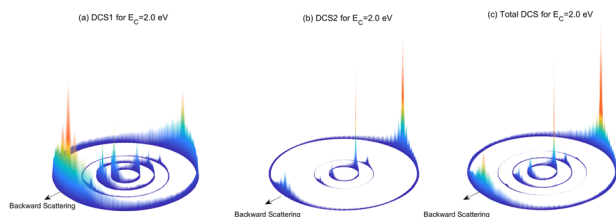
4845

## Ligand impacts on band edge energies and excited state splittings of silicane

Guoying Yao, Ekadashi Pradhan, Zhenyu Yang\* and Tao Zeng\*



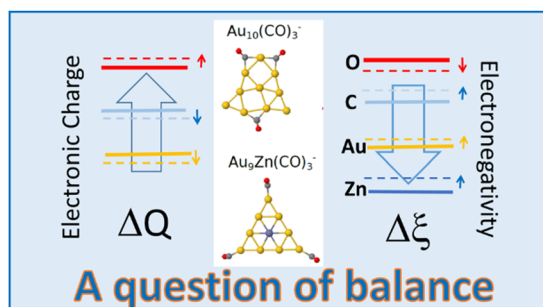
4858



### Quantum state-to-state dynamics of $C(^3P) + H_2(X^1\Sigma_g^+) \rightarrow CH(^2\Pi) + H(^2S)$ reaction based on a new $CH_2(X^3A'')$ potential energy surface

Juan Zhao, Daguang Yue, Dong Liu, Shang Gao, Lifei Wang and Lulu Zhang\*

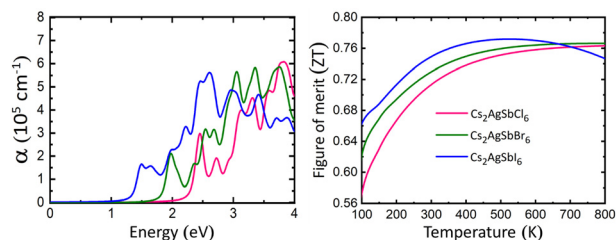
4871



### Sequential adsorption of multiple CO molecules on $Au_{10}^-$ and $Au_9Zn^-$ triangular clusters: the crucial role of a single atomic impurity

Eva M. Fernández\* and Luis C. Balbás

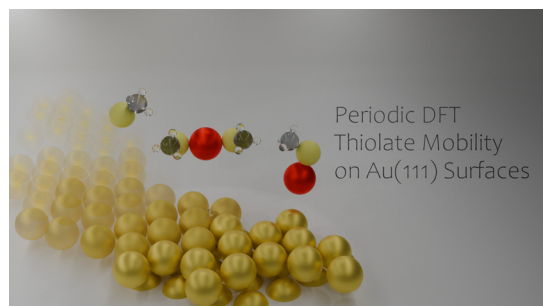
4880



### Exploring double perovskites $Cs_2AgSbX_6$ ( $X = Cl, Br, \text{ and } I$ ) as promising optoelectronic and thermoelectric materials: a first-principles study

Asim Sajjad, Muhammad Faizan,\* Tahani A. Alrebdi, Ghulam Murtaza, Javed Rehman, Xingchen Shen, Yujing Dong, Kausar Shaheen and Shah Haidar Khan\*

4892



### Mobility of thiolates on $Au(111)$ surfaces

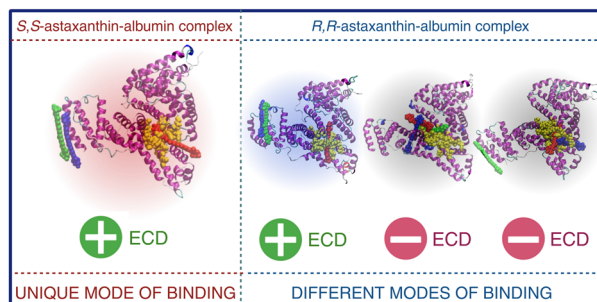
Daniël R. Duijnste, Moniek Tromp, Wesley R. Browne\* and Aleksandar Staykov\*



4905

### Enantiorecognition in a multi-component environment

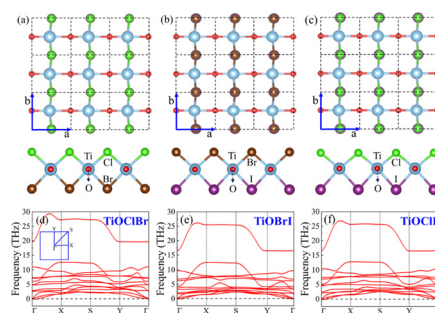
Joanna Mazurkiewicz, Ewa Stanek, Pedro Maximiano, Tiago H. Ferreira, Marta Karpiel, Szymon Buda, Justyna Kalinowska-Tłuścik, Pedro N. Simões, Igor Reva and Agnieszka Kaczor\*



4915

### Prediction of two-dimensional narrow-gap Janus $\text{TiOXY}$ ( $X, Y = \text{Cl, Br, I}; X \neq Y$ ) monolayers for electronic and optoelectronic applications

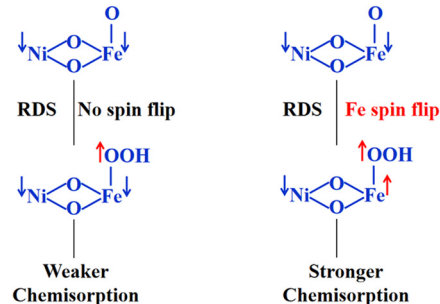
Yange Peng, Xiuwen Wu, Shengzhao Yang, Jiansheng Dong, Xi Fu, Hairui Bao\* and Wenhui Liao\*



4926

### Oxygen evolution reaction on NiFe-LDH/ $(\text{Ni,Fe})\text{OOH}$ : theoretical insights into the effects of electronic structure and spin-state evolution

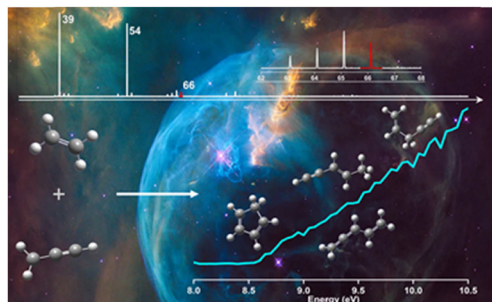
Qian Lin, Guangjun Nan, Dawei Fu and Liyan Xie\*



4934

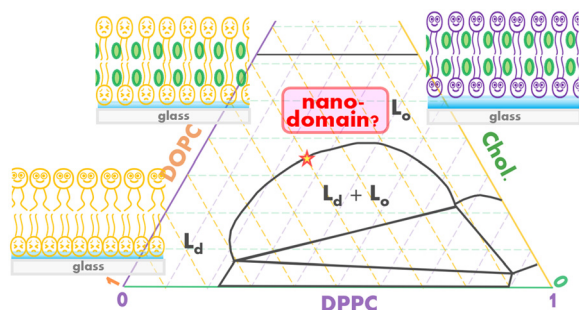
### Formation of $\text{C}_5\text{H}_6$ isomers: a combination of experimental and computational investigation

Yi-Fan Zhang, Wang Li,\* Chang-Yang Wang, Chen Huang, Hui-Ting Bian\* and Long Zhao\*



## RESEARCH PAPERS

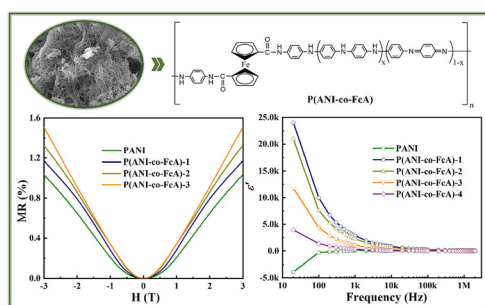
4944



### A macroscopically homogeneous lipid phase exhibits leaflet-specific lipid diffusion in a glass-supported lipid bilayer

Takuhiro Otsu,\* Miyuki Sakaguchi and Shoichi Yamaguchi

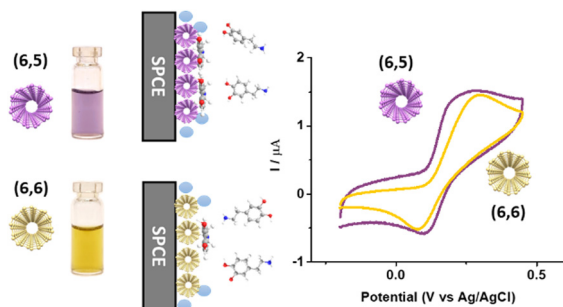
4950



### Ferrocene derivatives and aniline copolymers with tunable magnetoresistance and dielectric properties

Huiyan Ren and Hongbo Gu\*

4959

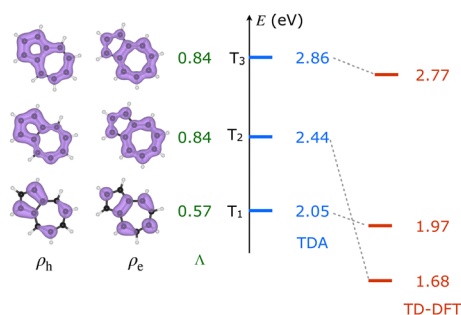


### Single-chirality single-wall carbon nanotubes for electrochemical biosensing

Ju-Yeon Seo, Bahar Mostafiz, Xiaomin Tu, Constantine Y. Khripin, Ming Zheng, Han Li\* and Emilia Peltola\*

## COMMENTS

4968



### Comment on "Designing potentially singlet fission materials with an anti-Kasha behaviour" by R. Pino-Rios, R. Báez-Grez, D. W. Szczepanik, and M. Solá, *Phys. Chem. Chem. Phys.*, 2024, 26, 15386

Komal Jindal, Atreyee Majumdar and Raghunathan Ramakrishnan\*

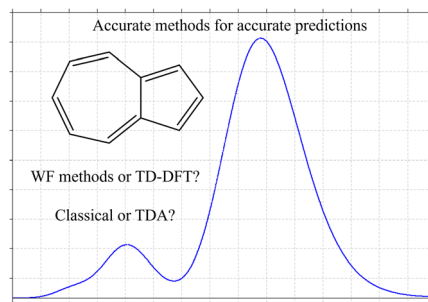


## COMMENTS

4973

Reply to the 'Comment on "Designing potentially singlet fission materials with an anti-Kasha behaviour"' by K. Jindal, A. Majumdar and R. Ramakrishnan, *Phys. Chem. Chem. Phys.*, 2025, 27, DOI: 10.1039/D4CP02863E

Ricardo Pino-Rios,\* Rodrigo Báez-Grez, Dariusz W. Szczepanik and Miquel Solà\*



## CORRECTION

4976

Correction: Designing potentially singlet fission materials with an anti-Kasha behaviour

Ricardo Pino-Rios,\* Rodrigo Báez-Grez, Dariusz W. Szczepanik and Miquel Solà\*

