

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(35) 18041–18798 (2025)



### Cover

See Enrique M. Arpa, pp. 18121–18127. Image reproduced by permission of Llum de Palau and Enrique M. Arpa from *Phys. Chem. Chem. Phys.*, 2025, 27, 18121. Image created by Llum de Palau (<https://lumdepalau.com>).



### Inside cover

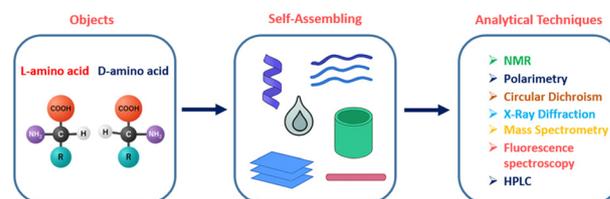
See Martin Schäfer and Karl-Michael Weitzel, pp. 18128–18140. Image reproduced by permission of Karl-Michael Weitzel from *Phys. Chem. Chem. Phys.*, 2025, 27, 18128.

## TUTORIAL REVIEW

18062

### Importance of chirality in the self-organizing peptides – from single molecules to functional supramolecular structures

Agata Chotera-Ouda, Katarzyna Trzeciak and Marek J. Potrzebowski\*

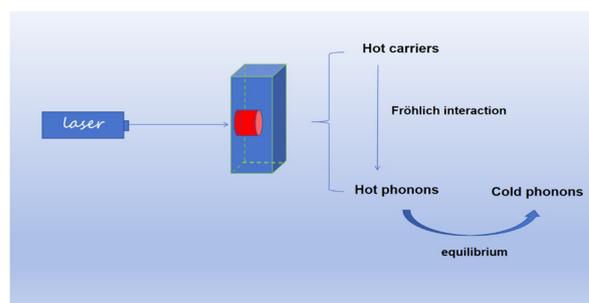


## PERSPECTIVE

18093

### Hot carriers and hot phonons in MAPbI<sub>3</sub> under pulsed excitation

Shuan Zhou, Chen-Guang Huang and Chen-Wu Wu\*



# Environmental Science: Atmospheres

GOLD  
OPEN  
ACCESS

Connecting communities  
and inspiring new ideas



Open Access Article. Published on 10 September 2025. Downloaded on 5/22/2026 1:23:16 AM.  
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

[rsc.li/submittoEA](https://rsc.li/submittoEA)

Fundamental questions  
Elemental answers

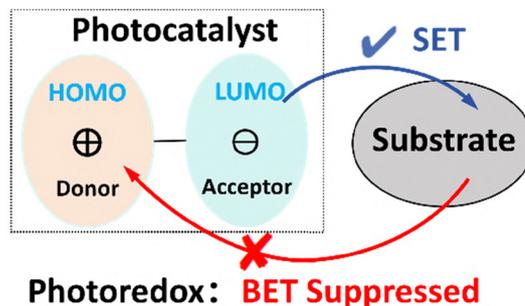


## COMMUNICATIONS

18107

### Intramolecular charge transfer state to suppress back electron transfer for singlet photoredox catalysis

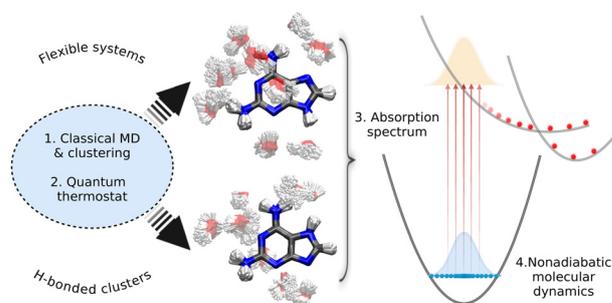
Yulong Ding and Shuming Bai\*



18112

### Investigating photodynamics of nucleobase–water systems

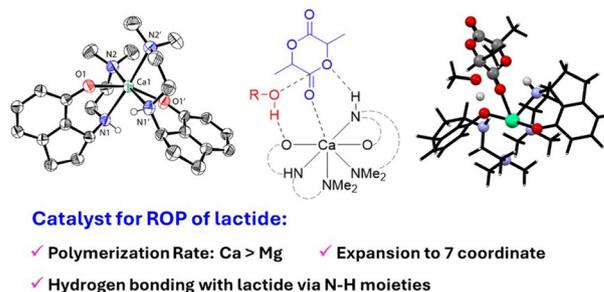
Haseena Sheik, Luca Grisanti, Tea Ostojić, Chaiyaporn Lakmuang, Barbara Rossi and Antonio Prlj\*



18116

### Homoleptic magnesium and calcium complexes supported by constrained reduced Schiff base ligand for lactide polymerisation: DFT analysis of lactide/ligand interactions

Trinity Quek, Thonthun Saeteaw, Tanyawan Pongpanit, Supawadee Namuangruk\* and Khamphee Phomphrai\*

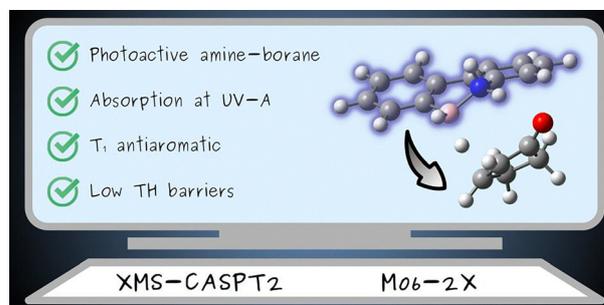


## RESEARCH PAPERS

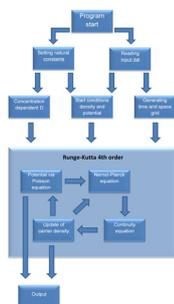
18121

### Excited-state antiaromaticity relief in photoactive amine–boranes promotes transfer hydrogenation to electron-poor olefins

Enrique M. Arpa



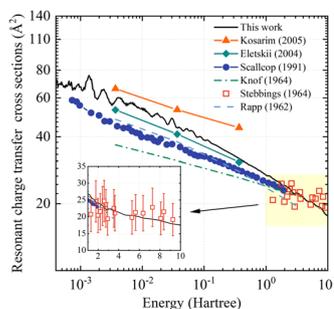
18128



## MAR\_CCT: Marburg program for modelling charge carrier transport

Martin Schäfer\* and Karl-Michael Weitzel\*

18141



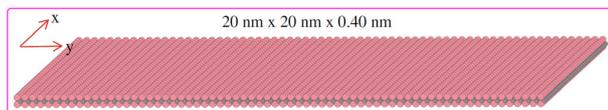
## Resonance charge exchange and collision integrals for $O(^3P)-O^+(^4S)$ and $O(^1D)-O^+(^4S)$ interactions

Zi Ding and Linhua Liu\*

18152

## Field-tunable skyrmion phases in monolayer MXene for spintronic applications

Junais Habeeb Mokkath\*



18162



## Molecular mobility and electrical conductivity of amino acid-based (DOPA) ionic liquid crystals in the bulk state and nanoconfinement

Mohamed A. Kolmangadi, Aileen R. Raab, Paulina Szymoniak, Zhuoqing Li, Patrick Huber, Sabine Laschat and Andreas Schönhals\*

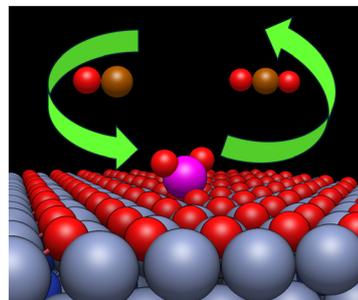


## RESEARCH PAPERS

18179

Single atom catalysts on the  $\text{Cr}_2\text{NO}_2$  MXene for CO oxidation

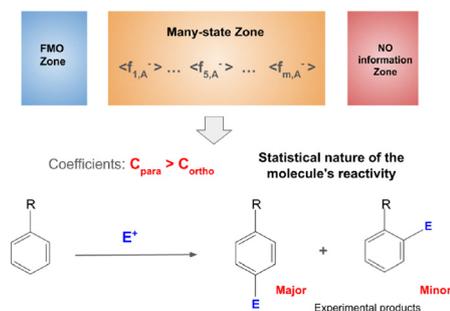
María Guadalupe Moreno-Armenta,\*  
Rodrigo Ponce-Perez, Francesc Viñes\* and  
Lourdes Mestres



18188

## A statistical theory of reactivity based on molecular orbitals participation and its application to organic reactions

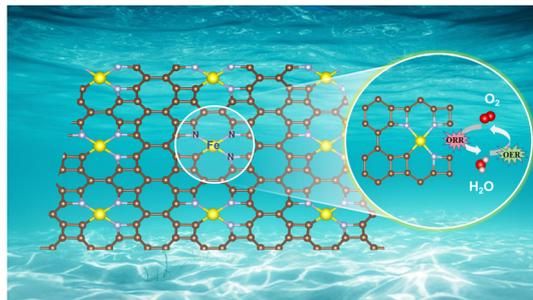
Javier Oller,\* Paul Geerlings, Frank De Proft and  
Pablo Jaque



18206

## The regulation of the bifunctional electrocatalytic activity of transition metal atoms embedded in a biphenylene network by the asymmetric nitrogen coordination environment

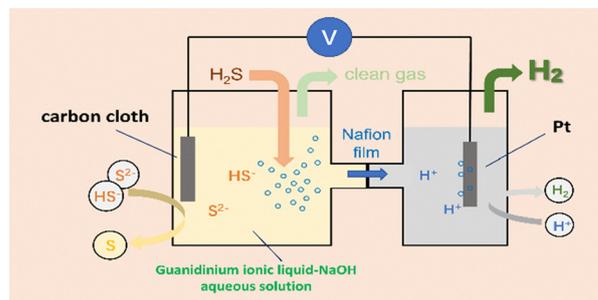
Lijia Luo, Zhengqin Zhao and Hui Wang\*



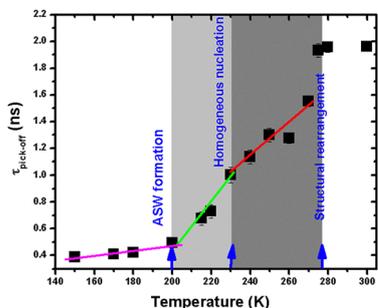
18214

Efficient capture and conversion of  $\text{H}_2\text{S}$  into  $\text{H}_2$  and sulfur in guanidinium ionic liquid–NaOH aqueous solution

Qianqian Peng, Chengxuan Zhou, Shucan Qin,  
Jinbiao Liang, Shengyun Xu, Jiaming Mao,  
Jianming Shi, Yanrong Liu\* and Yunqian Ma\*



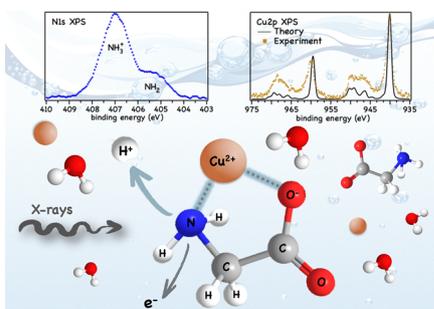
18222



### Amorphous solid water prevails inside the spherical nanopores of the MIL-101(Cr) framework below 200 K: PALS, XRD and BDS studies

Vivek Sudhir, Debarati Das, Pranav Utpalla, Siddhartha Kolay, Manvendra Narayan Singh and Dhanadeep Dutta\*

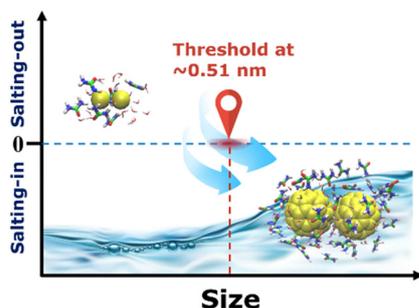
18234



### Revealing ligand deprotonation and speciation pathways in Cu(II)–glycine aqueous solutions via liquid-jet X-ray photoelectron spectroscopy supported by *ab initio* calculations

D. Céolin, T. Saisopa,\* Y. Rattanachai, S. Tangsukworakhun, W. Pokapanich, P. Songsirittigul, C. Songsirittigul, K. Klaiphet, J. Palaudoux, C. Nicolas and S. Carniato

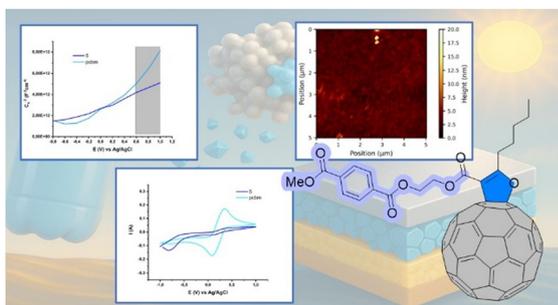
18248



### Size-dependent desolvation of hydrophobic nanoparticles in aqueous osmolytes

Bing Fang, Guochao Sun, Yuanyuan Qu, Yong-Qiang Li, Xiangdong Liu, Yanmei Yang\* and Weifeng Li\*

18256



### Early-stage analysis of PET – fullerene derivatives for electron transport in photovoltaics

Milica Đapović, Katarina Cvetanović, Vojislava Pošić, Vladislav Jovanov, Marko V. Bošković, Christos Polyzoidis, Nikolaos Tzoganakis, Konstantinos Rogdakis, Emmanuel Kymakis, Veselin Maslak\* and Aleksandra Mitrović\*

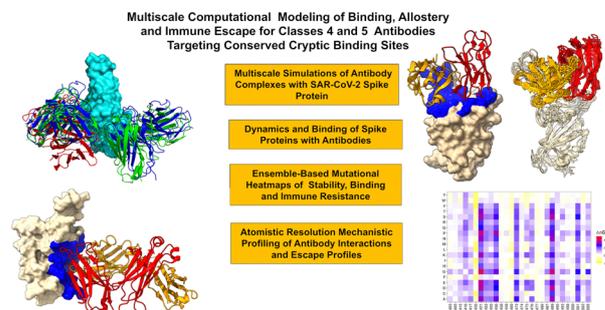


## RESEARCH PAPERS

18263

### Dynamic mutational profiling of binding interactions and allosteric networks in conformational ensembles of the SARS-CoV-2 spike protein complexes with classes of antibodies targeting cryptic binding sites: confluence of binding and allostery determines molecular mechanisms and hotspots of immune escape

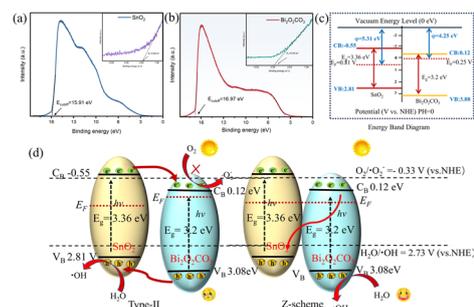
Mohammed Alshahrani, Vedant Parikh, Brandon Foley and Gennady Verkhivker\*



18288

### A pine cone-like $\text{SnO}_2/\text{Bi}_2\text{O}_2\text{CO}_3$ Z-scheme heterojunction photocatalyst enhances the photocatalytic degradation of tetracycline

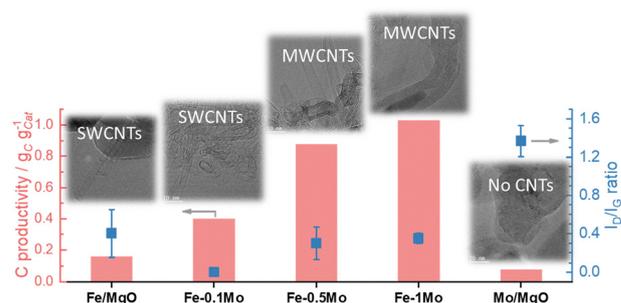
Xinyu Zheng, Shoufeng Zhang, Chen Liang, Peng Zhang, Jielu Yu,\* Che Zhang\* and Peng Gao\*



18302

### Tunable synthesis of carbon nanotubes *via* methane catalytic pyrolysis by adjusting Mo incorporation in Fe/MgO

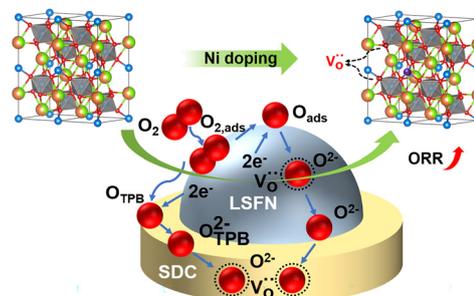
Zeyou Pan, Frank Krumeich, Paweł P. Ziemiański and Jeroen A. van Bokhoven\*



18309

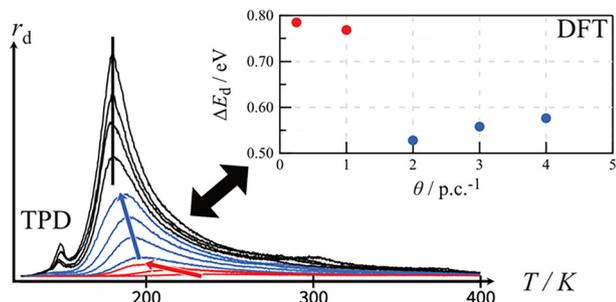
### Regulation of electronic and ionic transport in Ni-doped $\text{La}_{0.6}\text{Sr}_{0.4}\text{FeO}_{3-\delta}$ for enhanced oxygen reduction in intermediate-temperature solid oxide fuel cells

Yuanyuan Ma, Songbo Li,\* Zhen Yan, Shengli An, Hongli Qiao, Yanpeng Liu, Jing Zhang, Xu Zhang, Guangrui Zhang and Jing Zhao



## RESEARCH PAPERS

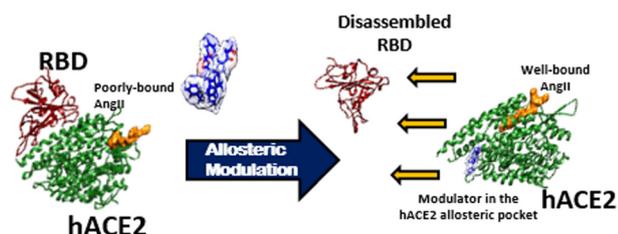
18317



### Water desorption from microcline (001): insights into the first water layer

Tobias Dickbreder,\* Florian Schneider, Lea Klausfering, Kim Noelle Dreier, Franziska Sabath, Adam S. Foster, Ralf Bechstein and Angelika Kühnle

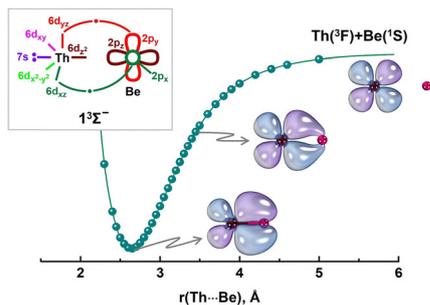
18326



### Modulating functional allostery of the host-cell receptor protein hACE2 to inhibit viral entry of SARS-CoV-2

Pratyush Pani, Saroj Kumar Panda and Malay Kumar Rana\*

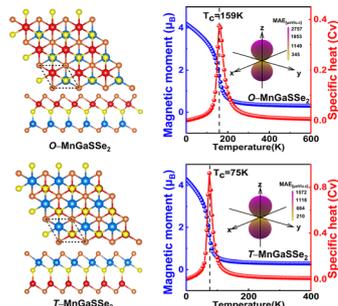
18341



### Ground and excited state properties of ThBe and AcBe

Isuru R. Ariyaratna

18351



### Possible transformation between half-metallic and metallic states of multiferroic MnGaSSe<sub>2</sub> monolayers

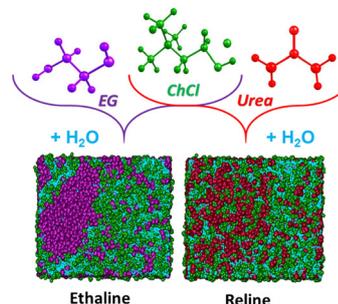
Zhiwen He, Shu Wang, Xue Rui, Jun Zhu, Yi Sun,\* Jinlian Lu, Xueke Yu\* and Xiuyun Zhang\*



18358

### Structural and interfacial behavior of choline chloride-based DESs (CholCl:EG and CholCl:urea) at various weight percentages in water mixture

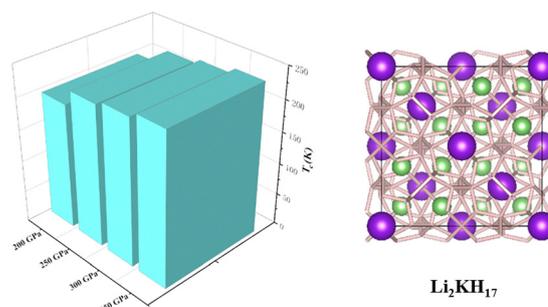
Rokhsareh Khodabandeh and Amin Reza Zolghadr\*



18379

### Superconducting properties of $\text{Li}_2\text{KH}_{17}$ with a cage configuration under high pressure

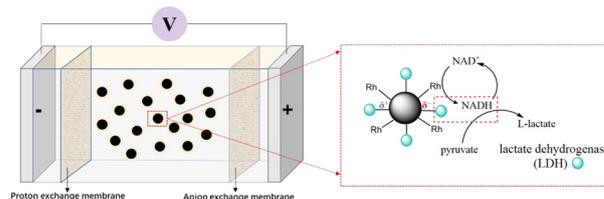
Qiyu Fu, Yuhang Wang, Xuejiao Xu, Wenhua Li, Xuyan Xue, Wei Zhang, Wencai Lu, Huijuan Sun\* and Wenhua Yang\*



18387

### Co-immobilization of a rhodium catalyst and LDH on a carbon electrode using a covalent graft strategy for electrocatalysis of L-lactate in a bipolar electrochemical system

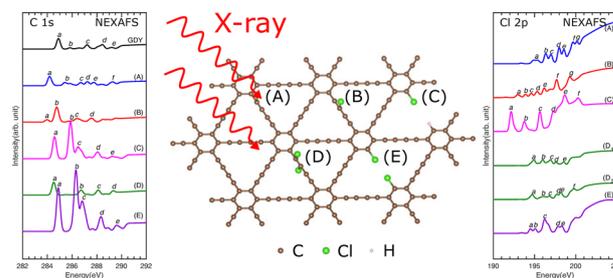
Chunhua Zhang,\* Bowen Li,\* Xiang Gao, Wei Xiao, Mingfang Chen and Qilong Bian\*



18395

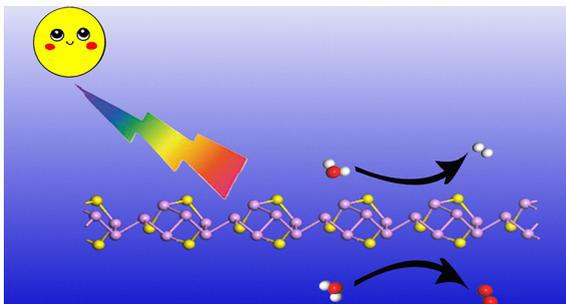
### Unveiling the structure of chlorine-doped graphdiyne via first-principles X-ray spectroscopy

Hao-Qing Zhu, Hai-Bo Li, Xiu-Neng Song and Yong Ma\*



## RESEARCH PAPERS

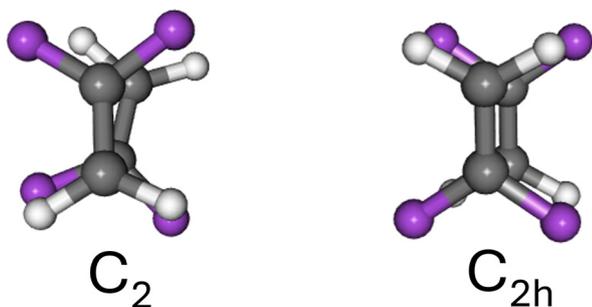
18403



### Two-dimensional P<sub>2</sub>S-I monolayer as a promising photocatalyst for overall water splitting

Xuan Li, Li Shao,\* Yanli Yang, Yuantao He, Yan Li and Jiehu Cui\*

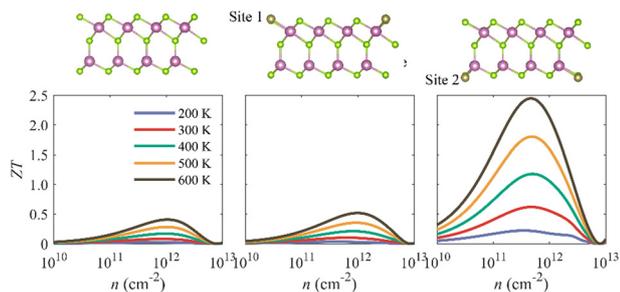
18409



### Low temperature jet spectra of (DFE)<sub>2</sub>, DFE-He, DFE-He<sub>2</sub> and DFE in the 2210–3105 cm<sup>-1</sup> region (DFE = 1,1 difluoroethylene)

A. J. Barclay, A. R. W. McKellar, A. Pietropolli Charmet and N. Moazzen-Ahmadi\*

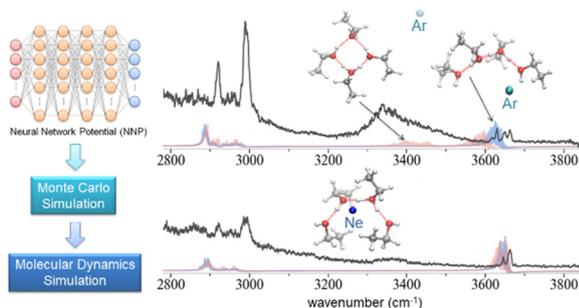
18420



### Boosting thermoelectric performance of ferroelectric monolayer $\alpha$ -In<sub>2</sub>Se<sub>3</sub> via strongly enhanced phonon scattering induced by site-specific Te doping

Weinan Zheng, Xinyang Li, Qiuyun Wang\* and Anmin Chen\*

18430



### Linear–cyclic isomer competition in protonated ethanol–methanol clusters probed by infrared spectroscopy and deep-learning structural and dynamical simulations

Po-Jen Hsu, Atsuya Mizuide, Jer-Lai Kuo\* and Asuka Fujii\*

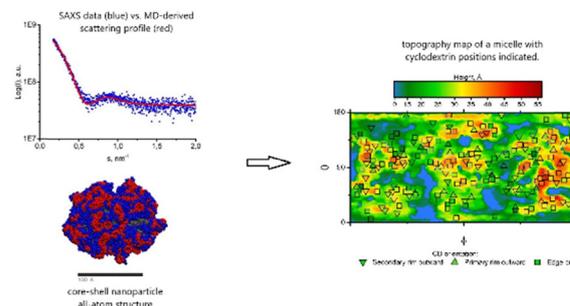


## RESEARCH PAPERS

18444

## Arrangement and dynamics of individual cyclodextrins on the surface of core-shell micelles

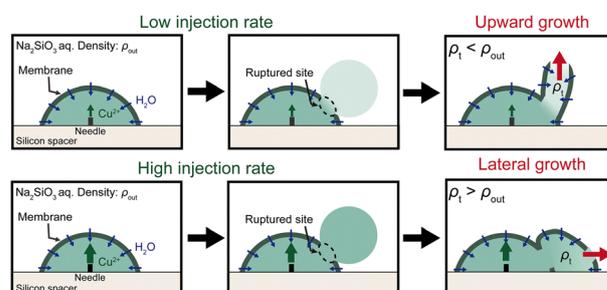
I. S. Vaskan,\* V. A. Dimitreva, A. A. Piryazev,  
E. N. Subcheva, N. V. Bovin, A. B. Tuzikov,  
V. A. Oleinikov and A. V. Zalygin\*



18454

## Injection rate control on the growth direction in chemical gardens

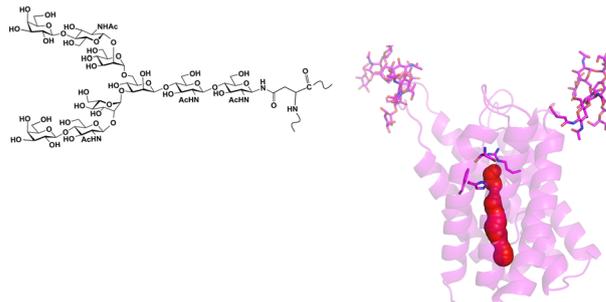
Yujin Kubodera, Muneyuki Matsuo and Satoshi Nakata\*



18459

## Mechanistic insights into glycosylation-driven structural rearrangements in human aquaporin 1

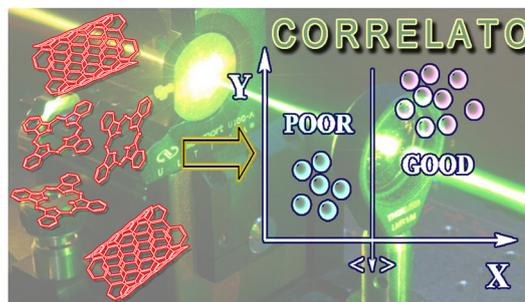
Keisuke Saito,\* Yasuhiro Kajihara\* and Hiroshi Ishikita\*



18467

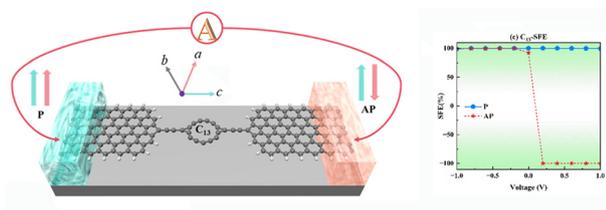
## Intelligent methods for assessing the efficiency of optical limiters based on carbon nanomaterials using the CORRELATO approach

Alexander Yu. Tolbin,\* Bogdan A. Tretyakov,  
Mikhail S. Savelyev, Pavel N. Vasilevsky and  
Alexander Yu. Gerasimenko



## RESEARCH PAPERS

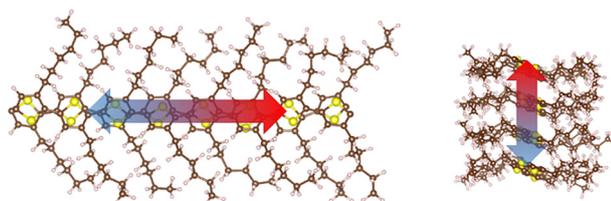
18478



### Spin multifunctional transport properties of $C_{13}$ and $C_{14}$ molecule-based molecular nanodevices

Shenlang Yan,\* Songbo Xiong, Tong Chen and Mengqiu Long

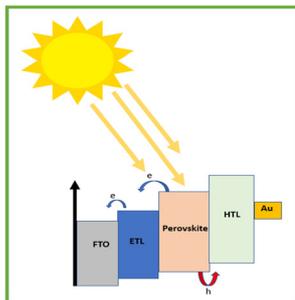
18487



### Heat transfer through covalent *versus* non-covalent bonding: a case study on crystalline $\pi$ -conjugated P3HT polymer using approach-to-equilibrium molecular dynamics

Cheick Oumar Diarra, Carlo Massobrio and Evelyne Martin\*

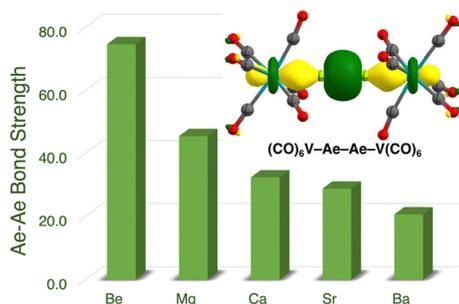
18496



### Impact of Ce doping on the optoelectronic and structural properties of a $CsPbI_2Br_2$ perovskite solar cell

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

18504



### Hepta-coordinated vanadium stabilized alkaline earth dimers: a DFT study

Ranjit Saha\* and Pratim Kumar Chattaraj\*

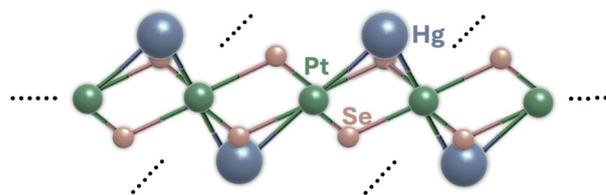


## RESEARCH PAPERS

18511

**Quantized optical conductivity of gated and irradiated monolayer  $\text{Pt}_2\text{HgSe}_3$** 

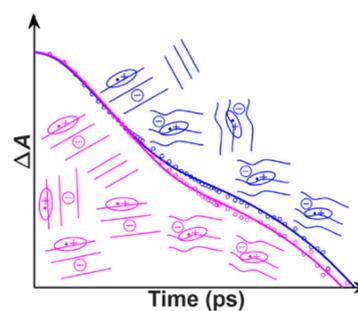
Bui D. Hoi\* and Ta T. Tho



18517

**Effect of local chain ordering on macroscopic charge mobility in chemically doped P3HT**

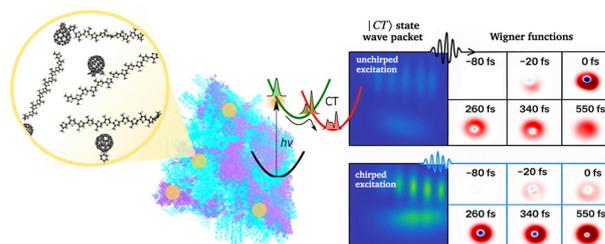
Abdul Rashid Umar, Adib Taba, Masoud Mahjouri-Samani and Christopher Grieco\*



18525

**Extending quantum coherence lifetimes in nonadiabatic dissipative molecular systems with chirped pulses**

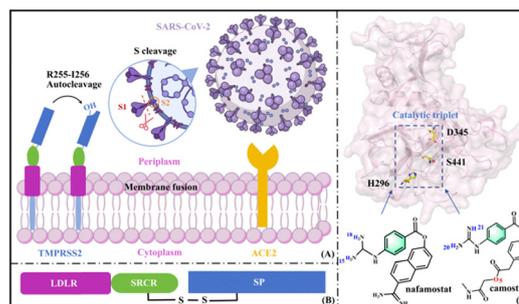
Robert Strich, Shirin Faraji and Elisa Palacino-González\*



18539

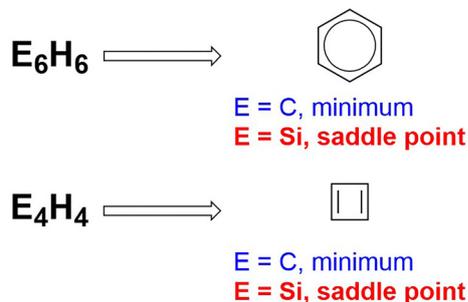
**Difference in the inhibitory mechanism against TMPRSS2 between camostat and nafamostat: implications for drug design**

Tiantian Yang, Wentong Yu, Du Guo, Jing Li, Xinmin Wang, Yuting Song, Yan Cheng, Yuxi Luo, Jianghua Yang, Weiwei Ouyang\* and Jianping Hu\*



## RESEARCH PAPERS

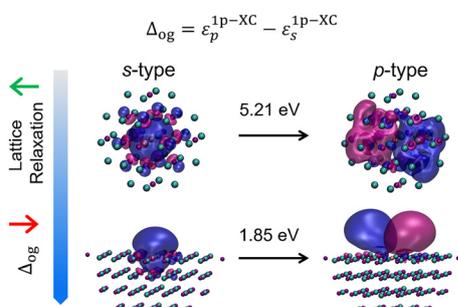
18555



**Aromaticity and antiaromaticity in the cyclic  $6\pi$  and  $4\pi$  molecules of carbon and silicon  $E_6H_6$  and  $E_4H_4$  (E = C, Si)**

Lili Zhao, Qin Ma, Israel Fernández\* and Gernot Frenking\*

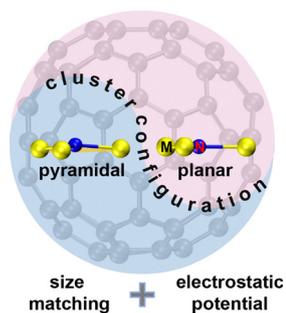
18567



**Optical gaps of F-center defects in LiF using many-body methods**

Ritaj Tyagi, Abhisek Ghosal and Vamsee K. Voora\*

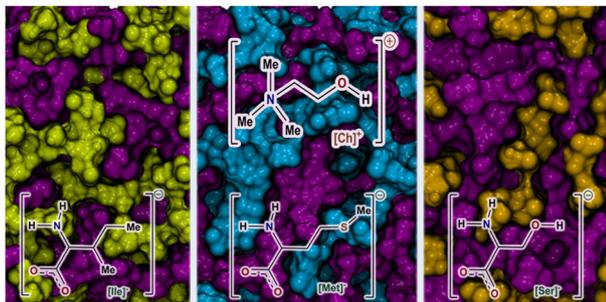
18577



**Size matching and electrostatic potential as complementary methods for understanding the metallic cluster configurations inside fullerenes**

Chenliang Pan, Shuaijiang Liu and Peng Jin\*

18586



**Tailoring ionic liquid properties via amino acid anions: structural influence of isoleucine, methionine, and serine anions**

Sonia Yadav and Anurag Prakash Sunda\*

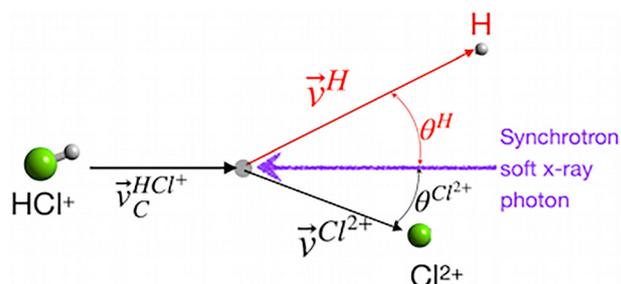


## RESEARCH PAPERS

18595

**Ionic photofragmentation cross sections of the  $\text{HS}^+$ ,  $\text{H}_2\text{S}^+$  and  $\text{HCl}^+$  molecular ions near the 2p threshold**

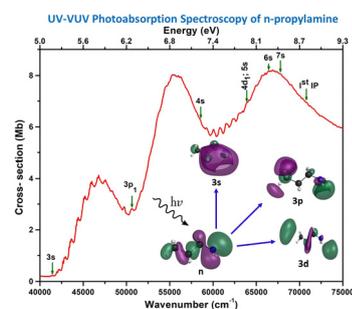
Jean-Paul Mosnier,\* Eugene T. Kennedy,  
Denis Cubaynes, Jean-Marc Bizau,  
Ségolène Guilbaud and Stéphane Carniato



18609

**UV-VUV absorption spectroscopy and photodissociation dynamics of *n*-propylamine**

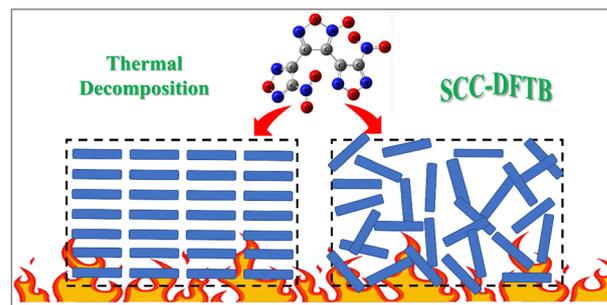
Neha Sharma, Aparna Shastri,\* Asim Kumar Das,  
Vandana Rawat and Balabhadrapatruni Naga Rajasekhar



18626

**Molecular packing-dependent thermal decomposition pathways in 3,4-dinitrofurazanfuroxan: insights from SCC-DFTB molecular dynamics simulations**

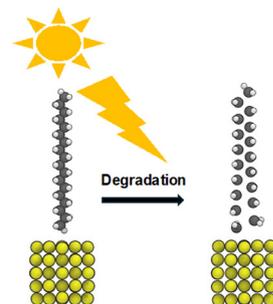
Shuangfei Zhu,\* Fangfang Hou, Jinxuan Xue,  
Ruijun Gou, Shuhai Zhang,\* Shangbiao Feng and  
Yang Liu



18635

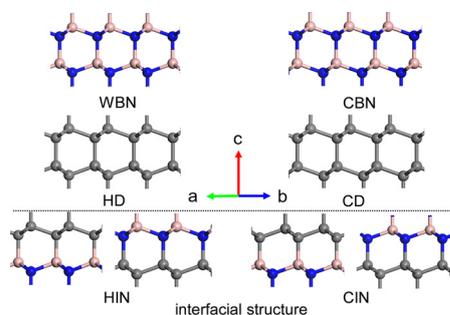
**Plasmonic degradation of plastics on gold nanoparticles: electronic-scale insights from computation**

Hajar Hosseini, Connor J. Herring, Noshir S. Pesika and  
Matthew M. Montemore\*



## RESEARCH PAPERS

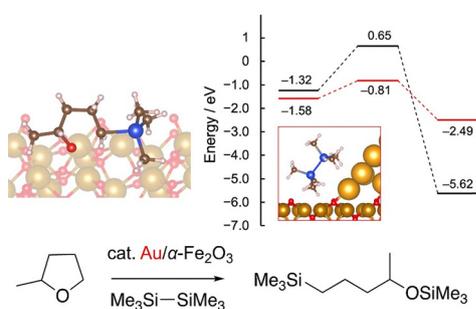
18645



### Examining the stability and mechanical characteristics of interface structures within diamond/BN composite materials

Qi Gao,\* Li Zhu, Kun Luo,\* Lingjuan Hao, Feifei Ling, Chao Ren, Xianda Han, Xiaogang Guo, Zhixuan Chen, Julong He and Dongli Yu

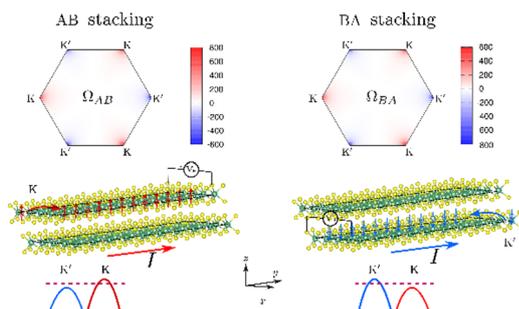
18651



### Reaction mechanism of silylation of C–O bonds in alkyl ethers over supported gold catalysts: experimental and theoretical investigations

Yunosuke Tsunesada, Tatsushi Ikeda, Koki Muraoka, Masafumi Doi, Hiroki Miura,\* Tetsuya Shishido\* and Akira Nakayama\*

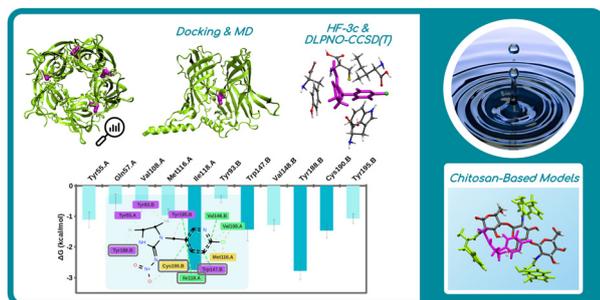
18658



### Electrically switchable valley polarization and an anomalous valley Hall effect in monolayer and bilayer NbS<sub>2</sub>

Zhifan Zheng, Tengfei Cao, Chun-Sheng Liu, Xiaohong Zheng,\* Hua Hao,\* Yushen Liu\* and Shaohui Yu

18665



### Towards nature-inspired materials for adsorbing pesticides: a multi-stage computational approach

J. R. C. Santos, P. E. Abreu and J. M. C. Marques\*

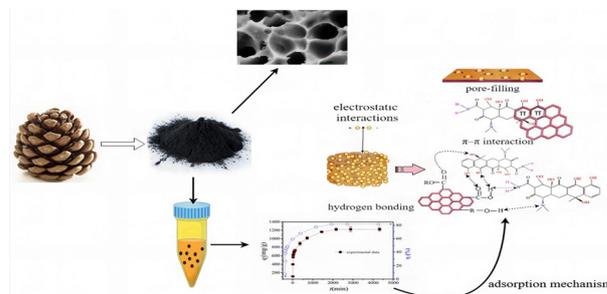


## RESEARCH PAPERS

18681

### Three-dimensional hierarchical porous P,O co-doped pinecone biochar for tetracycline removal: behavior and mechanism

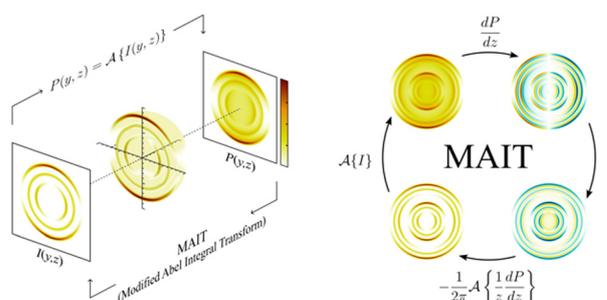
Jianfang Lu, Chaojie Fan, Yuanyuan Huang, Pengfei Li, Fuhou Lei, Haitang Xu, Caiyun Han, Kechun Li\* and Yu Feng\*



18694

### Revisiting the inverse Abel integral for reconstructing velocity-map images

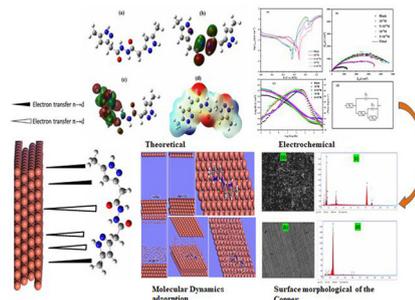
Chris Sparling\* and Jolijn Onvlee\*



18710

### Electrochemical and theoretical insights into Schiff base derivatives for the prevention of copper corrosion

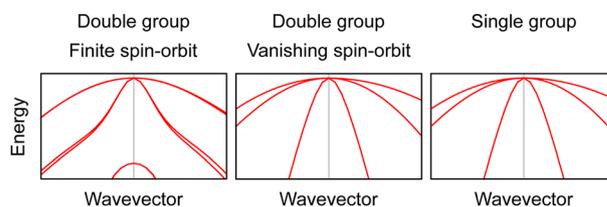
Mohammed Lasri,\* Abouelhaoul El Alami, Nouredine Idlahoussaine, Aziz Ait-Karra, Othmane Zakir, Mohamed Maatallah, Rachid Idouhli, Rabiaa Fdil, Mohy Eddine Khadiri and Abdesselam Abouelfida



18723

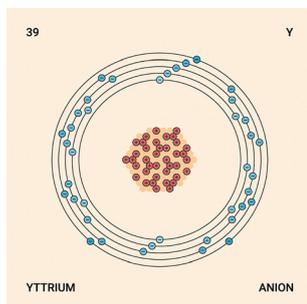
### Kramers degeneracy originates from two time-reversal symmetries

Koshi Okamura



## RESEARCH PAPERS

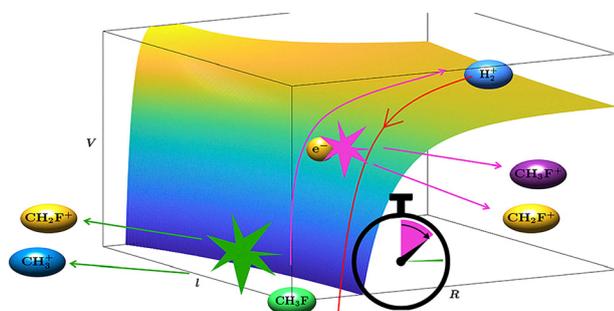
18734



### Understanding the binding in excited states of the yttrium anion

Maria Barysz

18741

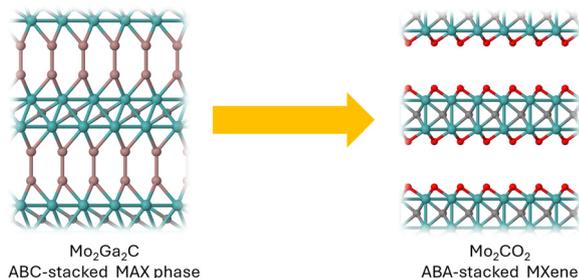


### Competition between electron transfer and reactive capture in ion–molecule reactions at low collision energies: isotopic and stereodynamic effects in the reactions of $\text{CH}_3\text{F}$ with $\text{H}_2^+$ , $\text{HD}^+$ and $\text{D}_2^+$

Raphaël Hahn, David Schlander, Jeremy O. Richardson, Timothy P. Softley and Frédéric Merkt\*

18760

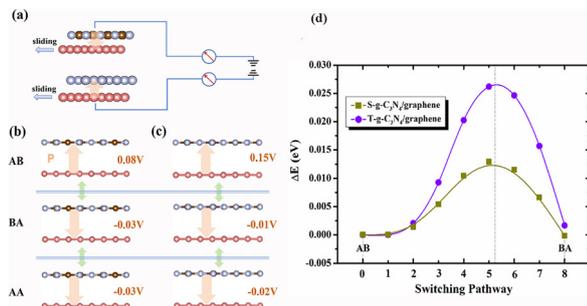
### Oxygen-aided Ga etching and ABC-to-ABA phase transition



### The role of oxygen in the synthesis of the $\text{Mo}_2\text{CT}_x$ MXene from the $\text{Mo}_2\text{Ga}_2\text{C}$ MAX phase

José D. Gouveia\* and José R. B. Gomes\*

18770



### Sliding ferroelectricity and alterpiezoelectricity in a two-dimensional heterobilayer from the in-plane hole of $g\text{-C}_3\text{N}_4$

Yuhua Wei, Feng Gao,\* XuLi Cheng, HaoTian Wang, YingJie Hu, ZuHui Hu, Hui Zhang, Jin Wen, Yin Wang\* and Wei Ren\*

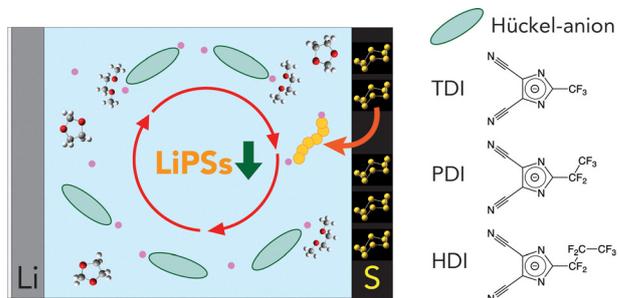


## RESEARCH PAPERS

18778

## Hückel anion based concentrated electrolytes for lithium–sulfur batteries

Aginmariya Kottarathil,\* N. Tan Luong, Carolina Cruz Cardona, Steffen Jeschke, Tomooki Hosaka, Grażyna Zofia Żukowska, Maciej Marczewski, Władysław Wiczorek and Patrik Johansson\*

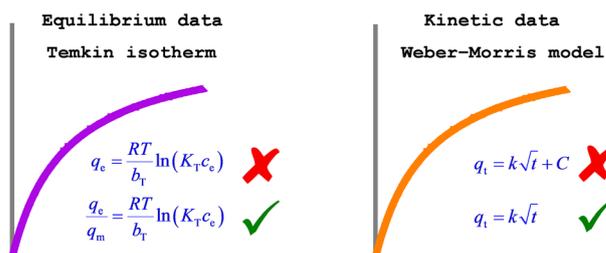


## COMMENTS

18789

Comment on “Unravelling the kinetics, isotherms, thermodynamics, and mass transfer behaviours of Zeolite Socony Mobil – 5 in removing hydrogen sulphide resulting from a dark fermentative biohydrogen production process” by M. K. A. Asman *et al.*, *Phys. Chem. Chem. Phys.*, 2024, 26, 20409

Khim Hoong Chu,\* Mohd Ali Hashim and Mohd Hafiz Zawawi

H<sub>2</sub>S adsorption on zeolite

18793

Reply to the ‘Comment on “Unravelling the kinetics, isotherms, thermodynamics, and mass transfer behaviours of Zeolite Socony Mobil – 5 in removing hydrogen sulphide resulting from a dark fermentative biohydrogen production process”’ by K. H. Chu, M. A. Hashim and M. Hafiz Zawawi, *Phys. Chem. Chem. Phys.*, 2025, 27, DOI: 10.1039/D4CP04682J

Muhammad Khairul Adha Asman, Nabilah Aminah Lutpi,\* Yee-Shian Wong, Soon-An Ong, Muhammad Adli Hanif, Naimah Ibrahim, Farrah Aini Dahalan, Wirach Taweepreda and Raja Nazrul Hakim Raja Nazri

