

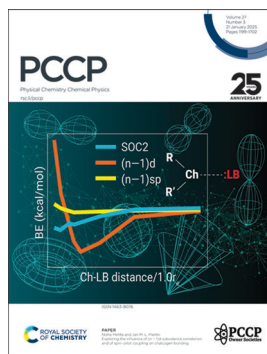
## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(3) 1199–1702 (2025)



### Cover

See Mercedes Alonso, Freija De Vleeschouwer *et al.*, pp. 1256–1273. Image reproduced by permission of Eline Desmedt & Michiel Jacobs from *Phys. Chem. Chem. Phys.*, 2025, 27, 1256.



### Inside cover

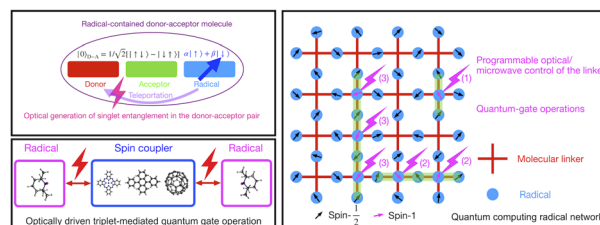
See Nisha Mehta and Jan M. L. Martin, pp. 1274–1283. Image reproduced by permission of Nisha Mehta and Jan M. L. Martin from *Phys. Chem. Chem. Phys.*, 2025, 27, 1274.

## REVIEW

1214

### Stable organic radicals – a material platform for developing molecular quantum technologies

Wei Wu

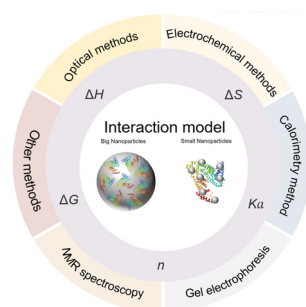


## PERSPECTIVE

1222

### Thermodynamics and models for small nanoparticles upon protein adsorption

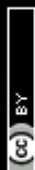
Miao-Miao Yin, Yi-Bo Yuan, Xin Ding, Yan-Jun Hu\* and Feng-Lei Jiang\*



# RSC Applied Polymers

The application of polymers,  
both natural and synthetic

Interdisciplinary and open access



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

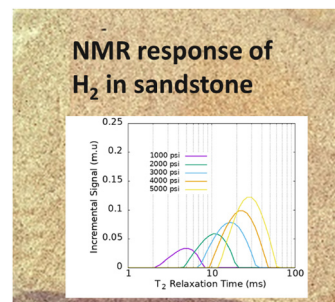
Fundamental questions  
Elemental answers

## COMMUNICATIONS

1237

### Evaluation of hydrogen storage in sandstone reservoirs using $^1\text{H}$ nuclear magnetic resonance spectroscopy

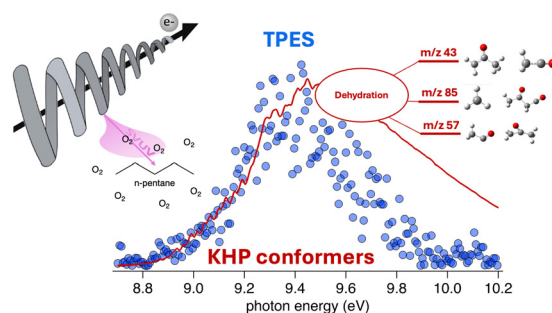
Son T. Dang,\* Sidi Mamoudou, Chandra S. Rai and Tuan A. Ho\*



1241

### Conformational effects in the identification and quantification of ketohydroperoxides in the oxidation of *n*-pentane

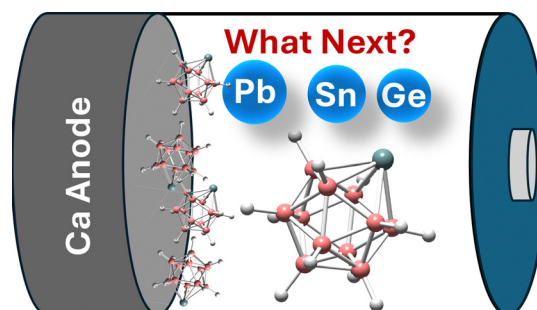
Dongyang Li, Deshan Li, Olivier Herbinet, Jiabin Huang, Gustavo A. Garcia, Philippe Arnoux, Luc-Sy Tran, Guillaume Vanhove, Laurent Nahon, Majdi Hochlaf, Hans-Heinrich Carstensen, Frédérique Battin-Leclerc, Julien Bloino, Feng Zhang\* and Jérémy Bourgalais\*



1250

### What comes next: the fate of germa-, stanna-, and plumba-closo-dodecaborate based electrolytes in calcium ion batteries

Mohmmad Faizan and Ravinder Pawar\*

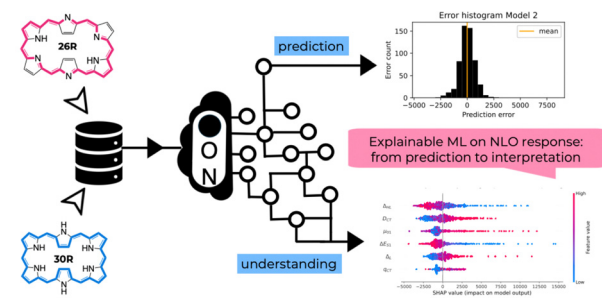


## RESEARCH PAPERS

1256

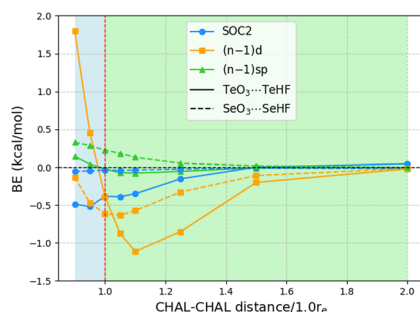
### Deciphering nonlinear optical properties in functionalized hexaphyrins via explainable machine learning

Eline Desmedt, Michiel Jacobs, Mercedes Alonso\* and Freija De Vleeschouwer\*



## RESEARCH PAPERS

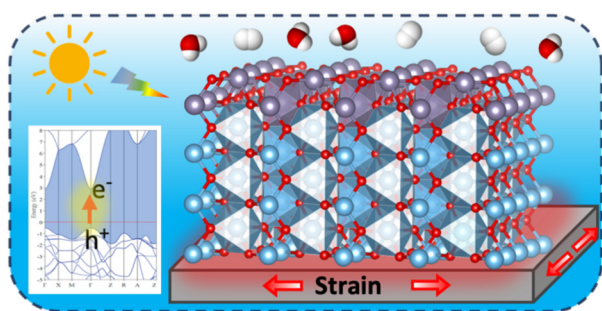
1274



### Exploring the influence of $(n - 1)d$ subvalence correlation and of spin-orbit coupling on chalcogen bonding

Nisha Mehta\* and Jan M. L. Martin

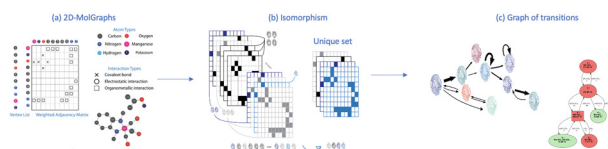
1284



### Enhancing the electronic and photocatalytic properties of $(\text{SnO}_2)_n/(\text{TiO}_2)_m$ oxide superlattices for efficient hydrogen production: a first-principles study

Najwa Harrati,\* Bastien Casier and Adlane Sayede\*

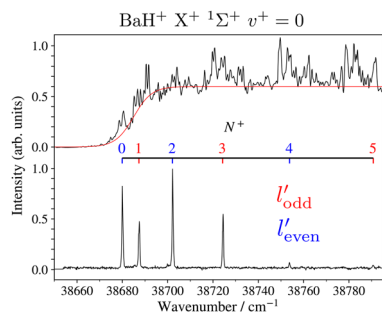
1298



### Exploiting graph theory in MD simulations for extracting chemical and physical properties of materials

Sana Bougueroua,\* Alexander A. Kolganov, Chloé Helain, Coralie Zens, Dominique Barth, Evgeny A. Pidko and Marie-Pierre Gaigeot\*

1310



### Characterisation of the electronic ground states of $\text{BaH}^+$ and $\text{BaD}^+$ by high-resolution photoelectron spectroscopy

J. R. Schmitz and F. Merkt\*

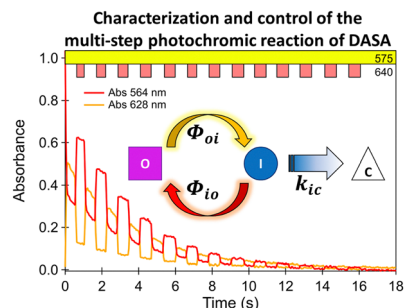


## RESEARCH PAPERS

1320

# Complete kinetic and photochemical characterization of the multi-step photochromic reaction of donor–acceptor Stenhouse adducts

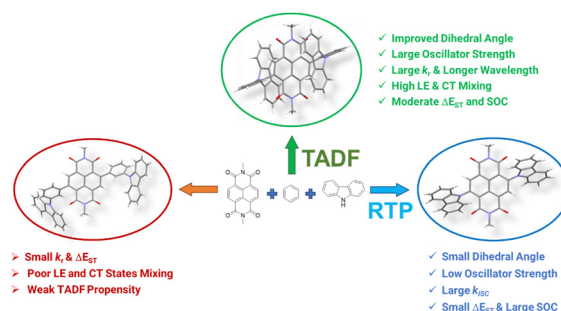
Julien Mallétroit, Aurélie Djian, Keitaro Nakatani, Juan Xie, Rémi Métivier\* and Guillaume Laurent\*



1327

# Theoretical elucidation of the effect of the linkage and orientation of carbazole and naphthalenediimide on the TADF and RTP propensities

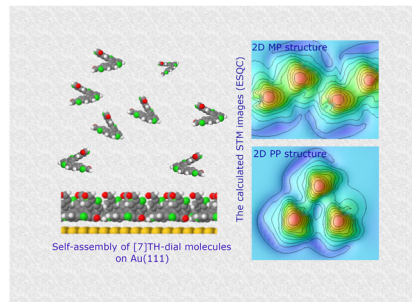
Chetan Saini, Siddan Gouthaman and K. R. Justin Thomas\*



1339

# Calculated and structural analyses of self-assembly formed by [7]thiaheterohelicene-2,13-carboxaldehyde molecules on Au(111)

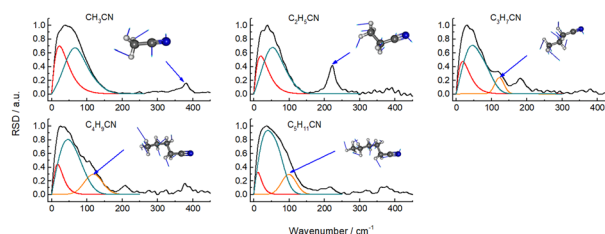
Nadia El Hasnaoui, Xavier Bouju and Youness Benjalal\*



1347

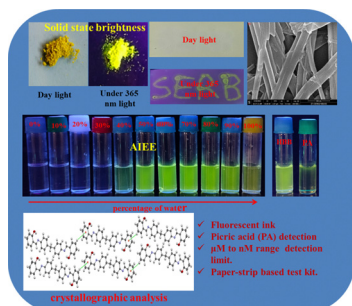
# Low-frequency (0–450 cm<sup>-1</sup>) dynamics of *n*-alkyl cyanide liquids studied by optical Kerr effect spectroscopy and density functional theory

Dujuan Meng, Sophia L. Sagala and Edward L. Quitevis\*



## RESEARCH PAPERS

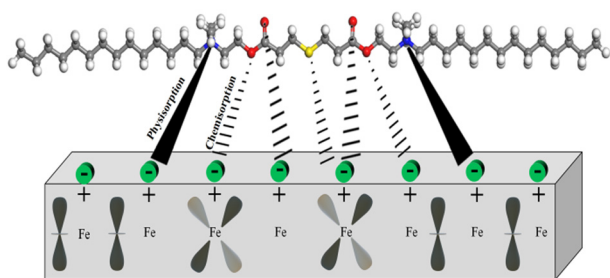
1366



**Brightness and AIEE behaviour of methylenebis(4,1-phenylene) linkage electron donor-acceptor-based dyads and their implications for robust quantification of explosive picric acid in both aqueous medium and solid state**

Manas Mahato, Tuhina Sultana, Rajkumar Sahoo, Sabbir Ahamed, Najmin Tohora, Arpita Maiti and Sudhir Kumar Das\*

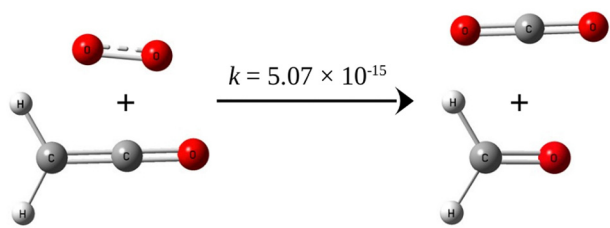
1378



**Experimental and computational studies of cationic Gemini surfactants as corrosion inhibitors for carbon steel in 15% HCl**

Chenxu Wang and Erlong Yang\*

1394

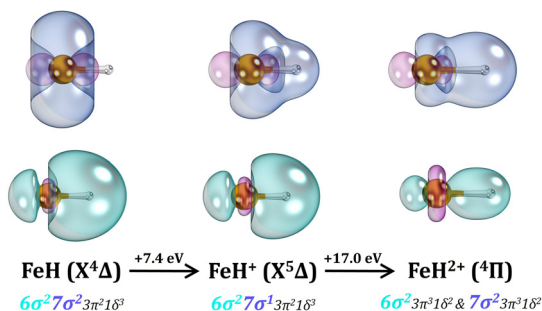


Rate coefficient in  $\text{cm}^3 \text{molecules}^{-1} \text{s}^{-1}$  at 298 K

**Singlet ( $^1\Delta_g$ )  $\text{O}_2$  initiated gas phase oxidation as a potential tropospheric decay channel for ketene**

Saptarshi Sarkar,\* Ashray Dhiman and Biman Bandyopadhyay\*

1402



**Ab initio electronic structures and total internal partition sums of  $\text{FeH}^{+/2+}$**

Isuru R. Ariyaratna,\* Jeffery A. Leiding, Amanda J. Neukirch and Mark C. Zammit

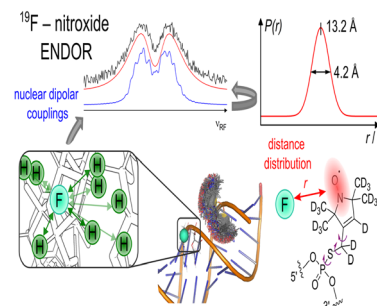


## RESEARCH PAPERS

1415

### Frequency and time domain $^{19}\text{F}$ ENDOR spectroscopy: role of nuclear dipolar couplings to determine distance distributions

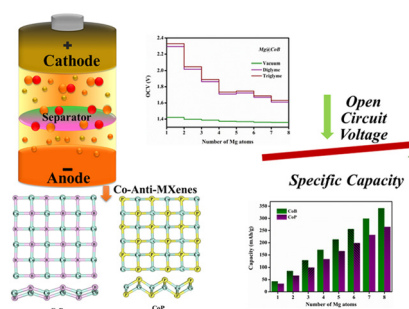
Annemarie Kehl,\* Lucca Sielaff, Laura Remmel,  
Maya L. Rämisch, Marina Bennati\* and Andreas Meyer\*



1426

### 2D Co-anti-MXenes (CoB/CoP) as promising anode materials for magnesium-ion batteries in diglyme and triglyme electrolytes: a first-principles study

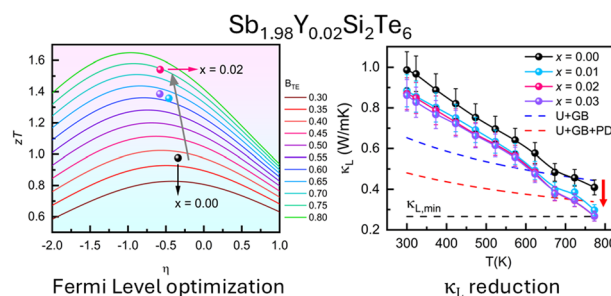
Nandhini Panjulingam and Senthilkumar Lakshmipathi\*



1437

### Improved thermoelectric efficiency of $\text{Sb}_2\text{Si}_2\text{Te}_6$ through yttrium-induced nanocompositing

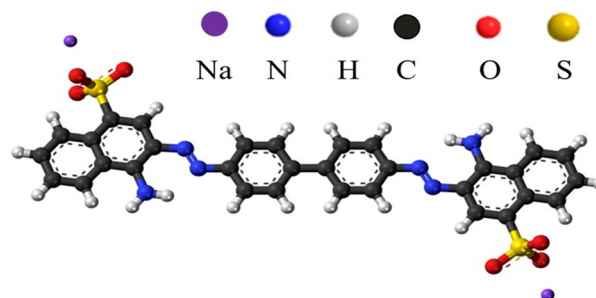
Kivanc Saglik, Xian Yi Tan, Jinfeng Dong, Ady Suwardi,  
Xizu Wang, Jianwei Xu, Qiang Zhu, Hongfei Liu,  
Jing Cao\* and Qingyu Yan\*



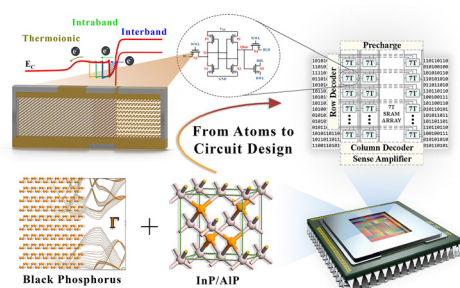
1447

### Nanostructured bismuth ferrite nanoparticles: synthesis, characterization, electrical/magnetic properties and photocatalytic performance

M. H. Ghozza, Ahmed T. Mosleh, Elbadawy A. Kamoun,\*  
Mahmoud Abdel-Aty, M. Alfiras, Mohamed Hafez Ahmed,  
Shawkat Alkhazaleh, V. Ganesh, H. Y. Zahran and  
Ibrahim S. Yahia\*



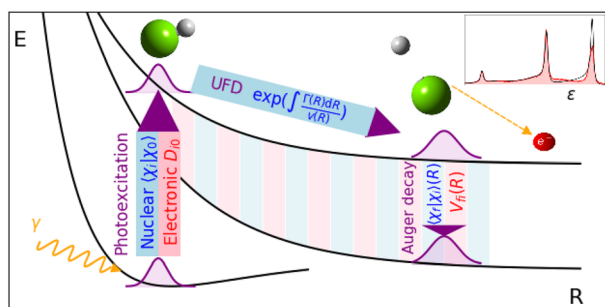
1459



### Phosphorus-based heterojunction tunnel field-effect transistors: from atomic insights to circuit renovations

Amir Khodabakhsh, Amir Amini\* and Arman Afzal

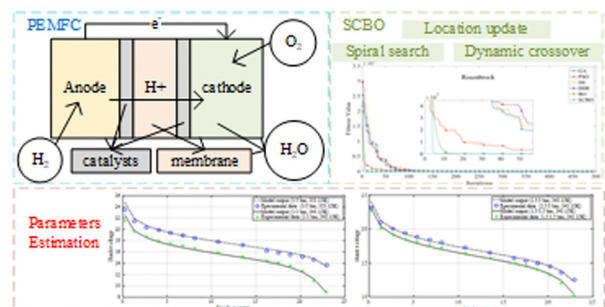
1473



### Ab initio Auger spectrum of the ultrafast dissociating $2p_{3/2}^{-1}\sigma^*$ resonance in HCl

Mateja Hrast\*, Marko Ljubotina and Matjaž Žitnik\*

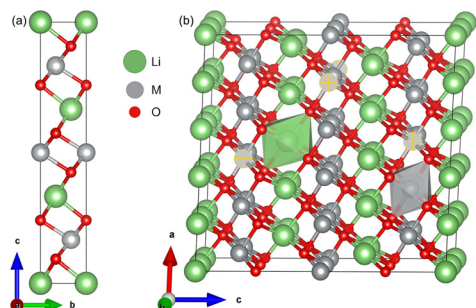
1483



### Estimation of PEMFC optimal parameters based on an improved butterfly optimization algorithm

Zhe Sun, Yan Song, Yijun Du and Zhixin Sun\*

1494



### Unlocking the potential of Ni-rich $\text{LiNi}_{0.9}\text{Co}_{0.1}\text{O}_2$ cathodes: a DFT investigation of performance-limiting factors

Temitayo Ojuetimi Ikuerowo, Olusegun Tomomewo and Salawu Omotayo Akande\*

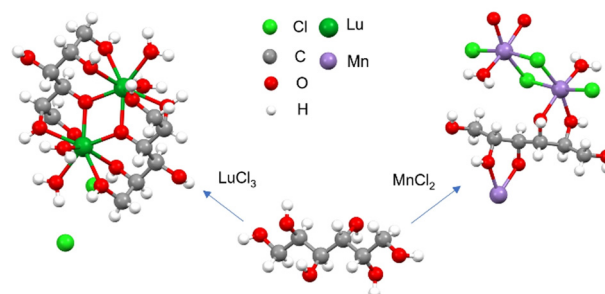


## RESEARCH PAPERS

1503

### Further exploration of the physicochemical nature of $\mu_2$ -bridge-relevant deprotonations *via* the elucidation of four kinds of alditol complexes

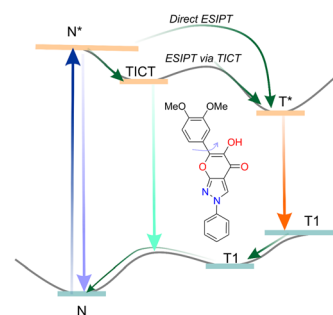
Yi Wu, Linchen Xie, Ye Jiang, Anqi He, Da Li,\*  
Limin Yang,\* Yizhuang Xu,\* Kexin Liu, Yukihiro Ozaki and  
Isao Noda



1515

### Concurrent ultrafast twisting and proton transfer photoreactions in new pyrano[2,3-*c*]pyrazole derivatives

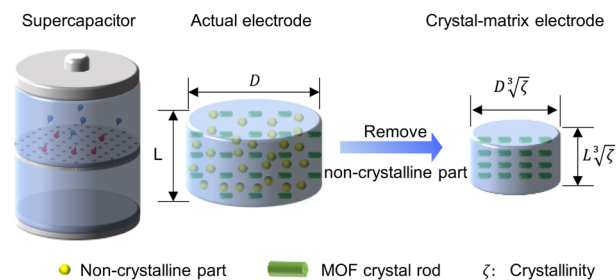
Marius Navickas,\* Karolis Gineitis, Arminas Urbonavičius,  
Sonata Krikštolė, Vytas Martynaitis, Eglė Arbačiauskienė,  
Miglė Dagilienė, Algirdas Šačkus and Mikas Vengris



1525

### A multi-scale circuit model bridges molecular modeling and experimental measurements of conductive metal–organic framework supercapacitors

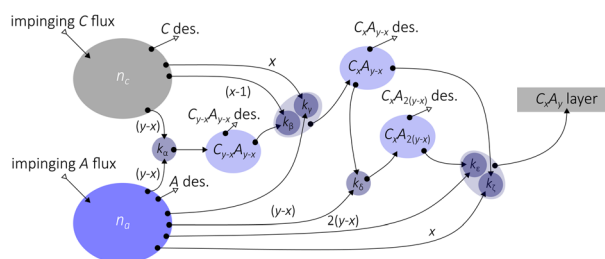
Liang Niu, Zhou Liu, Ding Yu, Volker Presser, Ming Chen  
and Guang Feng\*



1534

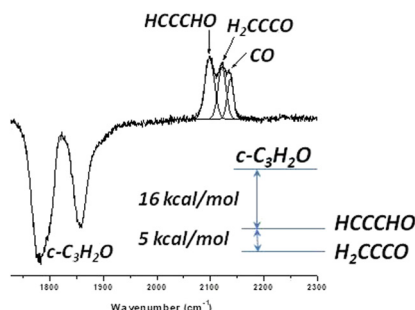
### Suboxides and subselenides: intermediate reaction products to form $\text{Ga}_2\text{O}_3$ , $\text{Ga}_2\text{Se}_3$ , $\text{In}_2\text{O}_3$ , $\text{In}_2\text{Se}_3$ , $\text{SnO}_2$ , and $\text{SnSe}_2$ during molecular-beam epitaxy

Patrick Vogt,\* Shun-Li Shang and Zi-Kui Liu



## RESEARCH PAPERS

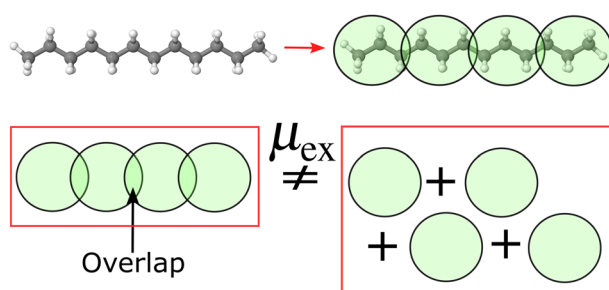
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### VUV photochemistry of cyclopropenone ( $c\text{-C}_3\text{H}_2\text{O}$ ): formation rate and abundance ratios of propynal ( $\text{HCCCHO}$ ) and propadienone ( $\text{CH}_2\text{CCO}$ )

Mohamad Ibrahim, Jean-Claude Guillemin and Lahouari Krim\*

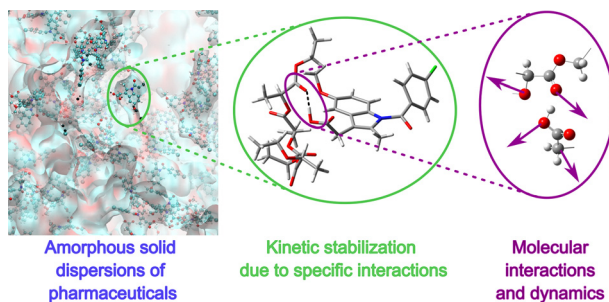
1554



### Dissipative particle dynamics parametrisation using infinite dilution activity coefficients: the impact of bonding

Rachel L. Hendrikse,\* Carlos Amador and Mark R. Wilson

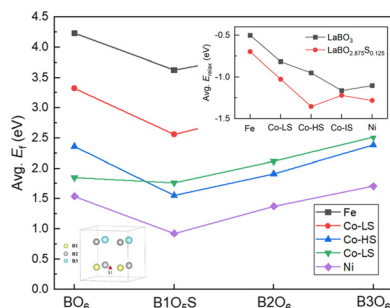
1567



### Molecular insights into kinetic stabilization of amorphous solid dispersion of pharmaceuticals

Vladislav Aulich, Jan Ludík, Michal Fulem and Ctirad Červinka\*

1585



### Sulfur-doping effects on oxygen vacancy formation in $\text{LaBO}_3$ ( $\text{B} = \text{Fe}, \text{Co}, \text{and Ni}$ ) perovskites

Ting Jia,\* Yinuo Hao and Hua Hao\*

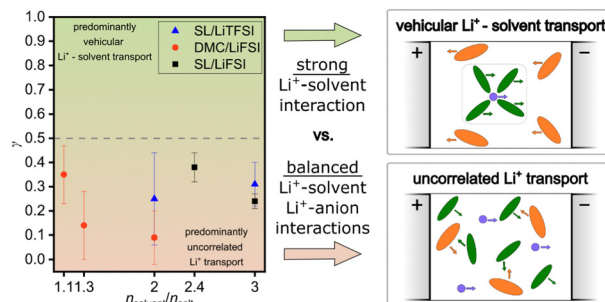


## RESEARCH PAPERS

1593

### Quantification of vehicular *versus* uncorrelated $\text{Li}^+$ -solvent transport in highly concentrated electrolytes *via* solvent-related Onsager coefficients

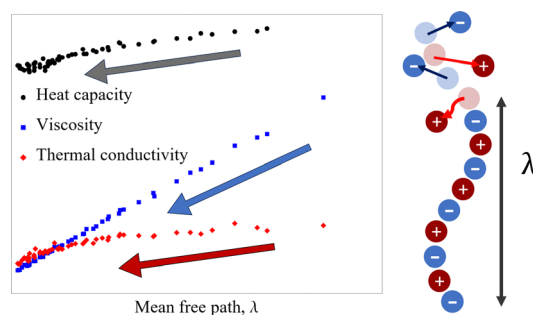
Hendrik Kilian, Tabita Pothmann, Martin Lorenz, Maleen Middendorf, Stefan Seus, Monika Schönhoff\* and Bernhard Roling\*



1604

### Thermodynamics and transport in molten chloride salts and their mixtures

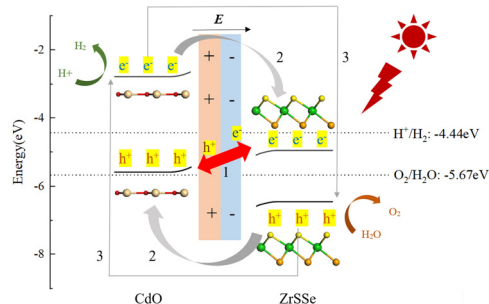
C. Cockrell,\* M. Withington, H. L. Devereux, A. M. Elena, I. T. Todorov, Z. K. Liu, S. L. Shang, J. S. McCloy, P. A. Bingham and K. Trachenko



1616

### First-principles investigation of the photocatalytic properties of two-dimensional CdO/ZrS<sub>2</sub> heterojunctions

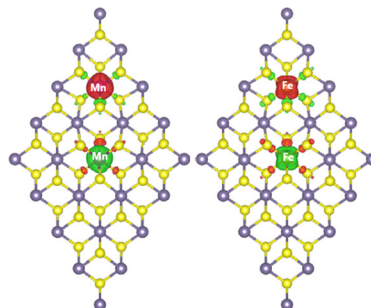
Deming Ma,\* Xiaohan Hui, Xiaoyu Yang, Yuhui Fu, Zhen Cui, Lin Zhang, Weili Ji, Yang Shen and Enling Li



1631

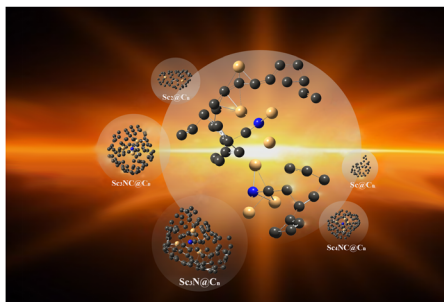
### Antiferromagnetic semiconductor nature in a GeS<sub>2</sub> monolayer doped with Mn and Fe transition metals

Vo Van On, Huynh Thi Phuong Thuy, J. Guerrero-Sanchez and D. M. Hoat\*



## RESEARCH PAPERS

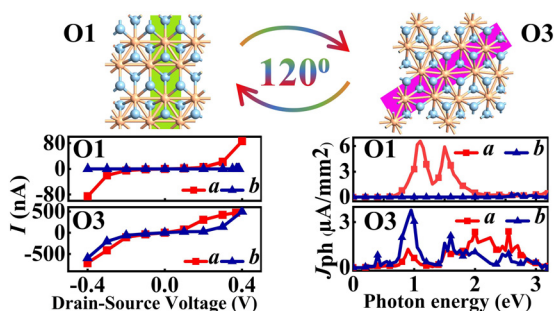
1640



# The formation mechanism of metal cluster fullerenes $\text{Sc}_3\text{N@C}_n$ : force field development and molecular dynamics simulations

Huichen Fan, Li-Hua Gan\* and Chun-Ru Wang

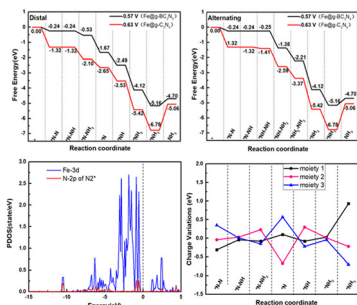
1648



# Ferroelastic phase transition-modulated electronic transport and photoelectric properties in monolayer 1T' ZrCl<sub>2</sub>

Yuehua Xu,\* He Sun, Jindian Chen, Qianqian Long and Haowen Xu

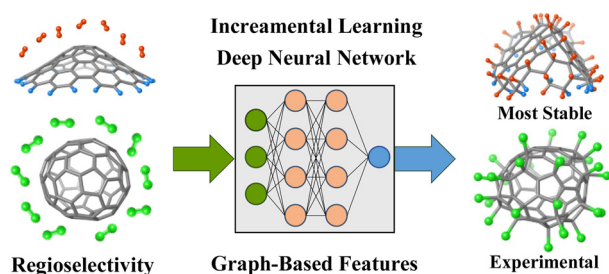
1661



# Single-atom transition metals supported on B-doped $\text{g-C}_3\text{N}_4$ monolayers for electrochemical nitrogen reduction

Huadou Chai, Weiguang Chen, Yi Li, Mingyu Zhao, Jinlei Shi, Yanan Tang\* and Xianqi Dai\*

1672



# Deep learning-driven prediction of chemical addition patterns for carboncones and fullerenes

Zhengda Li, Xuyang Chen and Yang Wang\*



1691

## Motility-induced collapse of an active Brownian particle polymer chain

Aleksandr Buglakov,\* Vasilisa Lelecova and Aleksandr Chertovich

