

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(32) 21307–21916 (2024)



### Cover

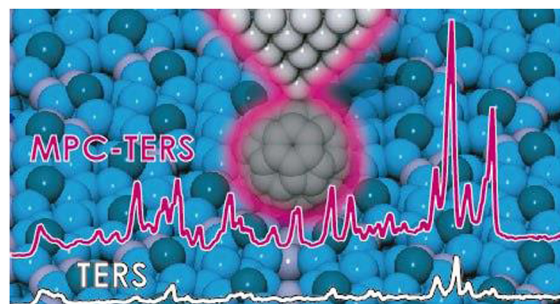
See Xiaoyang Liu, Vyacheslav S. Bryantsev, Anatoly I. Frenkel, Yu-chen Karen Chen-Wiegart *et al.*, pp. 21342–21356. Image reproduced by permission of Yu-chen Karen Chen-Wiegart from *Phys. Chem. Chem. Phys.*, 2024, 26, 21342.

## COMMUNICATIONS

21325

### Single-molecule tip-enhanced Raman spectroscopy of C<sub>60</sub> on the Si(111)-(7 × 7) surface

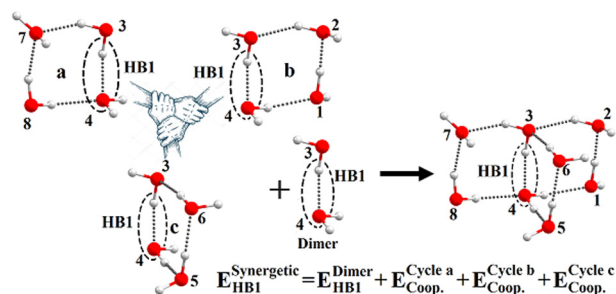
Borja Cirera,\* Shuyi Liu, Youngwook Park, Ikutaro Hamada, Martin Wolf, Akitoshi Shiotari and Takashi Kumagai



21332

### On the synergetic effects of cyclic cooperativity in water clusters

Ayush Shivhare, Bharti Dehariya, Shridhar R. Gadre and Milind M. Deshmukh\*



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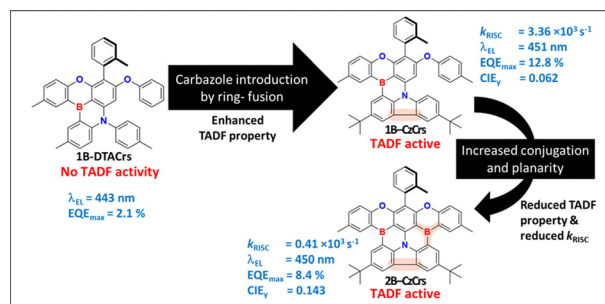
Fundamental questions  
Elemental answers

## COMMUNICATIONS

21337

### Molecular asymmetry and rigidification as strategies to activate and enhance thermally activated delayed fluorescence in deep-blue MR-TADF emitters

Rangani Wathsala Weerasinghe, John Marques dos Santos, Youhei Chitose, Tomas Matulaitis, Stuart L. Warriner, Debasish Barman, Chin-Yiu Chan,\* Youichi Tsuchiya,\* Eli Zysman-Colman\* and Chihaya Adachi\*

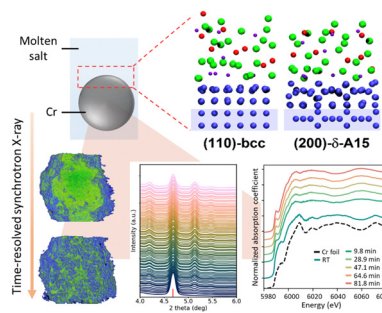


## RESEARCH PAPERS

21342

### Exploring Cr and molten salt interfacial interactions for molten salt applications

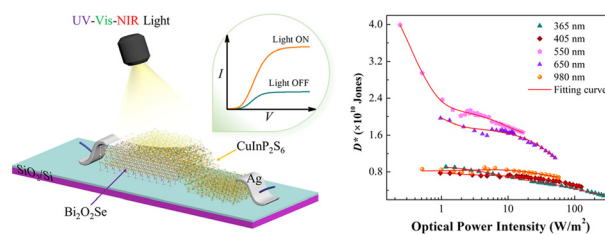
Xiaoyang Liu, Yang Liu, Luke D. Gibson, Mingyuan Ge, Daniel Olds, Denis Leshchev, Jianming Bai, Anna M. Plonka, Phillip Halstenberg, Hui Zhong, Sanjit Ghose, Cheng-Hung Lin, Xiaoyin Zheng, Xianghui Xiao, Wah-Keat Lee, Sheng Dai, German D. Samolyuk, Vyacheslav S. Bryantsev,\* Anatoly I. Frenkel\* and Yu-chen Karen Chen-Wiegart\*



21357

### Enhanced photoelectric performance of $\text{Bi}_2\text{O}_2\text{Se}/\text{CuInP}_2\text{S}_6$ heterojunction via ferroelectric polarization in two-dimensional $\text{CuInP}_2\text{S}_6$

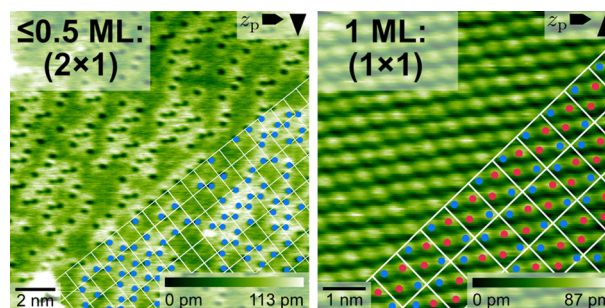
Di Wang, Qiong Wu, Kaihan Shan, Mengwei Han, Wenyu Jiang, Weiting Meng, Yanqing Zhang and Weiming Xiong\*



21365

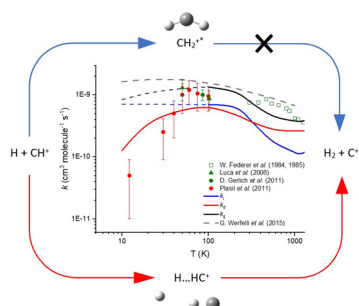
### Water adsorption lifts the $(2 \times 1)$ reconstruction of calcite(104)

Jonas Heggemann, Simon Aeschlimann, Tobias Dickbreder, Yashasvi S. Ranawat, Ralf Bechstein, Angelika Kühnle, Adam S. Foster\* and Philipp Rahe\*



## RESEARCH PAPERS

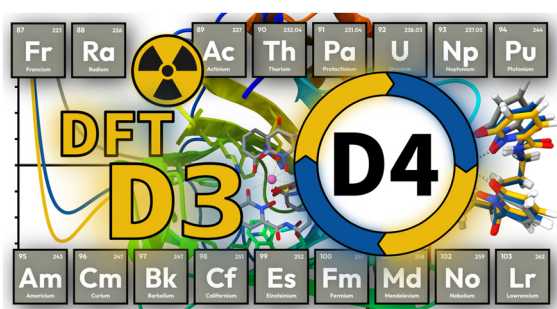
21370



### The temperature variation of the $\text{CH}^+ + \text{H}$ reaction rate coefficients: a puzzle finally understood?

Rafael A. Jara-Toro, Octavio Roncero and François Lique\*

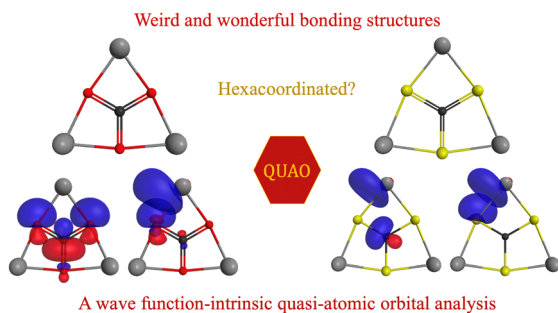
21379



### Extension of the D3 and D4 London dispersion corrections to the full actinides series

Lukas Wittmann, Igor Gordiy, Marvin Friede, Benjamin Helmich-Paris, Stefan Grimme, Andreas Hansen\* and Markus Bursch\*

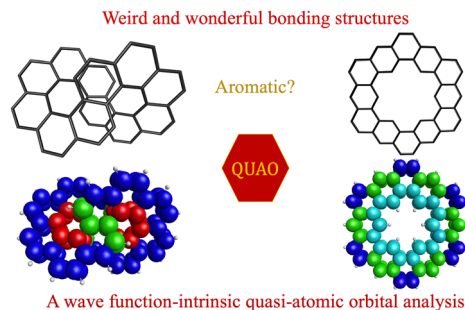
21395



### Analysis of bonding motifs in unusual molecules I: planar hexacoordinated carbon atoms

Daniel Del Angel Cruz, Katherine N. Ferreras, Taylor Harville, George Schoendorff and Mark S. Gordon\*

21407



### Analysis of bonding motifs in unusual molecules II: infinitene

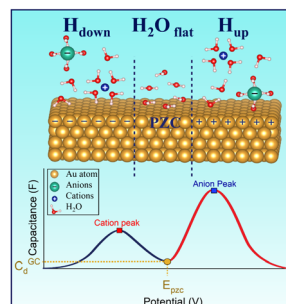
Katherine N. Ferreras, Taylor Harville, Daniel Del Angel Cruz and Mark S. Gordon\*



21419

### Tracking the surface structure and the influence of cations and anions on the double-layer region of a Au(111) electrode

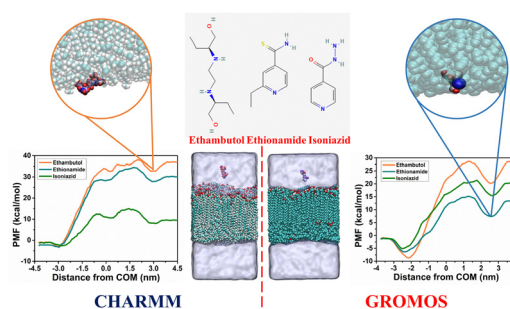
Ariba Adnan, Saeid Behjati, Núria Féllez-Guerrero, Kasinath Ojha and Marc T. M. Koper\*



21429

### Permeability of TB drugs through the mycolic acid monolayer: a tale of two force fields

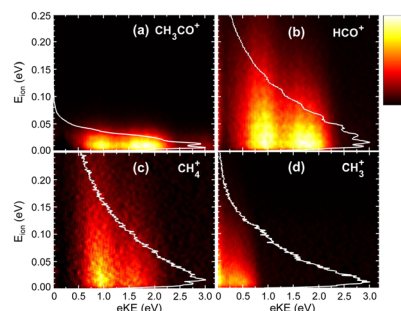
Subhadip Basu, Sandip Mandal and Prabal K. Maiti\*



21441

### Dissociative photoionization of acetaldehyde in the 10.2–19.5 eV VUV range

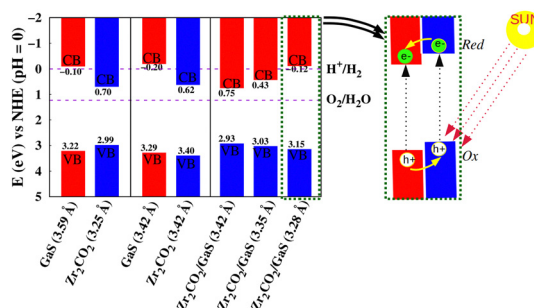
Pedro Recio, Roger Y. Bello, Gustavo A. García, Alexandre Zanchet, Jesús González-Vázquez, Luis Bañares and Sonia Marggi Poullain\*



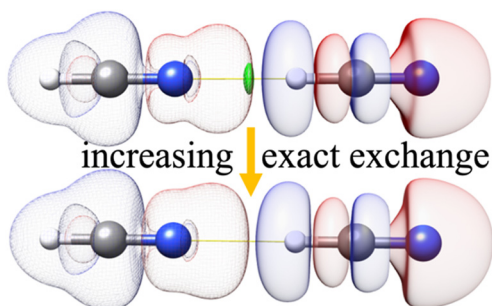
21453

### Exploring the properties of Zr<sub>2</sub>CO<sub>2</sub>/GaS van der Waals heterostructures for optoelectronic applications

Altaf Ur Rahman,\* Muhammad Abdul,\* Altaf Karim, Gul Rahman,\* Islam H. El Azab and Bao Jingfu



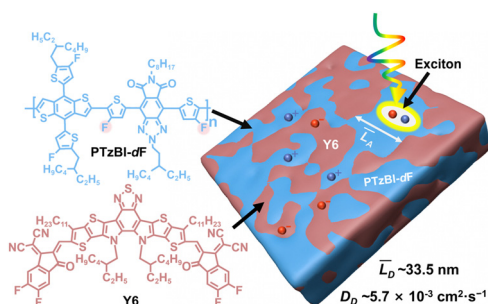
21468



### Spurious proton transfer in hydrogen bonded dimers

Joanatan Bautista-Renedo\* and Joel Ireta\*

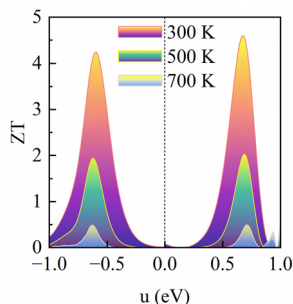
21476



### Charge photogeneration and recombination dynamics in non-fullerene solar cells based on a polymer donor with a mono-fluorinated $\pi$ -bridge

Haobo Lin, Zijie Xiao, Chuan Chen, Zekai Cai, Yuan Liang\* and Wei Zhang\*

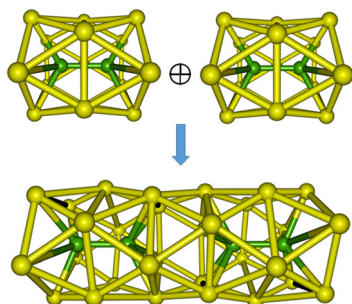
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### Ultralow lattice thermal conductivity and excellent thermoelectric performance of monolayer CdGaInS<sub>4</sub>: a first-principles investigation

Fanguang Kuang,\* Shuying Kang,\* Wei Huang, Yongqiang Xu and Yu Qi

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### The smallest triple-ring tubular gold clusters M<sub>2</sub>@Au<sub>15</sub> with M = Mo, W: stability, electronic properties and nonlinear optical response

Nguyen Thi Bao Trang, Minh Triet Dang, Nguyen Thanh Si, Tran Thi Ngoc Thao, Pham Thi Bich Thao, Minh Tho Nguyen\* and Pham Vu Nhat\*

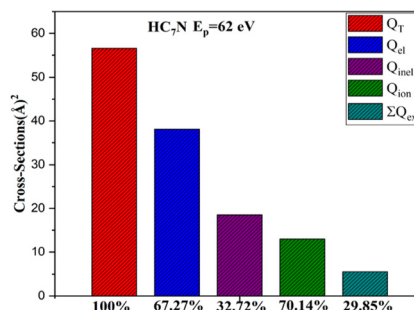


## RESEARCH PAPERS

21504

Electron-driven molecular processes for cyanopolyacetylenes  $\text{HC}_{2n+1}\text{N}$  ( $n = 3, 4,$  and  $5$ )

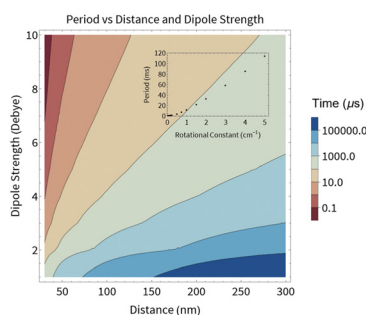
Pinal Mer and Chetan Limbachiya\*



21513

## Alignment transport between ultracold polar molecules

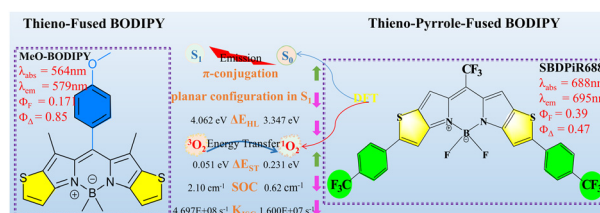
Jonathan Smucker\* and Jesus Pérez-Ríos



21520

## Theoretical study on the photophysical properties of thiophene-fused-type BODIPY series molecules in fluorescence imaging and photodynamic therapy

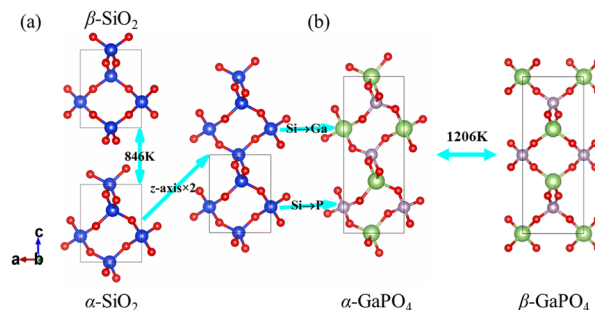
Jianfang Cao,\* Xinyu Chen, Xue Ma, Tianci Zhang and Wen Sun\*



21530

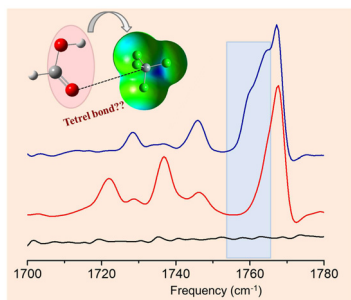
*Ab initio* study of temperature-dependent piezoelectric and electronic properties of thermally stable  $\text{GaPO}_4$ 

Xiaoqing Yang, Pan Guo, Shunbo Hu, Zhibin Gao, Wenliang Yao, Jinrong Cheng, Samuel Poncé, Baigeng Wang and Wei Ren\*



## RESEARCH PAPERS

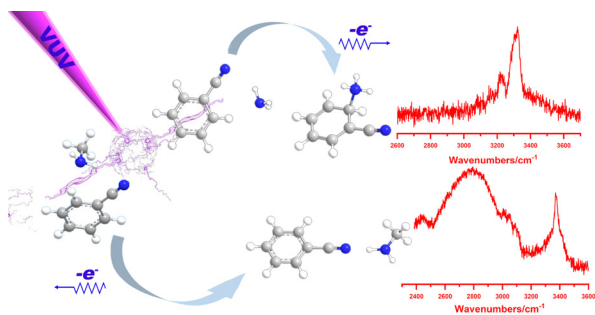
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**From 'halogen' to 'tetrel' bonds: matrix isolation IR spectroscopic and quantum mechanical studies of the effect of central atom substitution in donor tetrahalogens on binary complex formation with formic acid**

Indrani Bhattacharya and Pujarini Banerjee\*

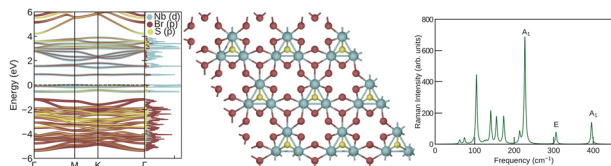
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**Growth mechanism of aromatic prebiotic molecules: insights from different processes of ion–molecule reactions in benzonitrile–ammonia and benzonitrile–methylamine clusters**

Xutao Chen, Yujian Li, Min Xie\* and Yongjun Hu\*

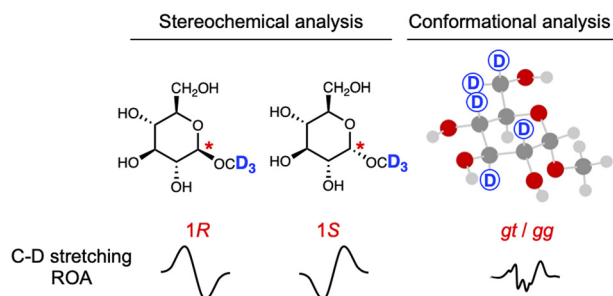
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**Exploring flat-band properties in two-dimensional  $M_3QX_7$  compounds**

Hai-Chen Wang, Tomáš Rauch, Andres Tellez-Mora, Ludger Wirtz, Aldo H. Romero\* and Miguel A. L. Marques\*

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**Raman optical activity study of deuterated sugars: deuterium labelling as a tool for structural analysis**

Tohru Taniguchi,\* Davidson Obinna Agbo, Qin Yang, Josef Kapitán, Tao Wu, Shuki Oyama, Shuji Akai, Yoshinari Sawama and Petr Bouř\*

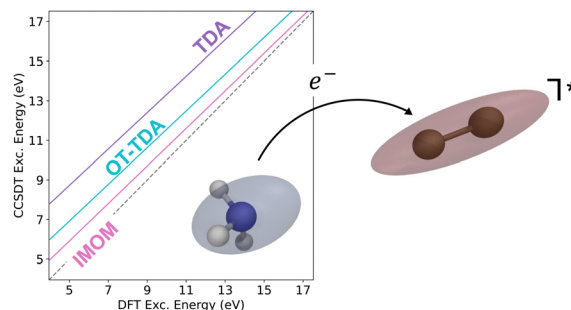


## RESEARCH PAPERS

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**Benchmarking DFT-based excited-state methods for intermolecular charge-transfer excitations**

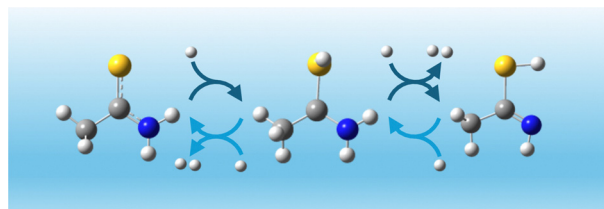
Nicola Bogo\* and Christopher J. Stein



21589

**Hydrogen-atom-assisted processes on thioacetamide in *para*-H<sub>2</sub> matrix – formation of thiol tautomers**

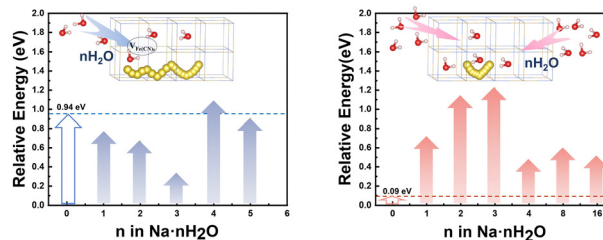
Sándor Góbi,\* Barbara Keresztes, Anita Schneiker and György Tarczay



21598

**Effect of water molecules on the diffusion of alkali metal ions in CuHCF cathodes**

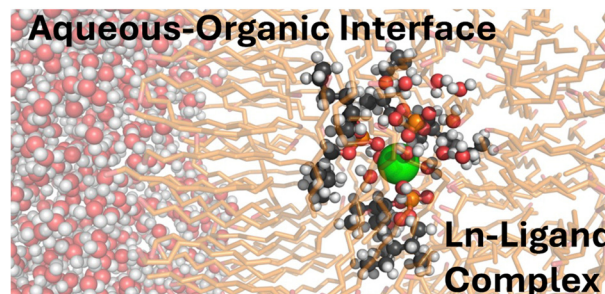
Silei Wang and Xiao Gu\*



21612

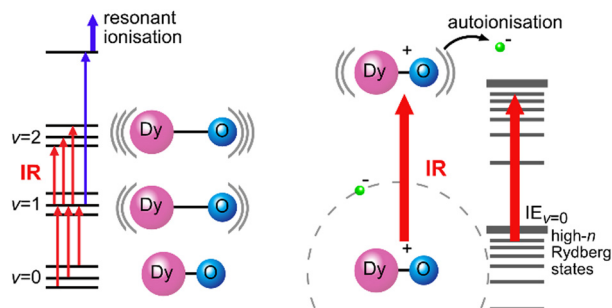
**Effect of ion to ligand ratio on the aqueous to organic relative solubility of a lanthanide–ligand complex**

Thomas J. Summers, Jesus Diaz Sanchez and David C. Cantu\*



## RESEARCH PAPERS

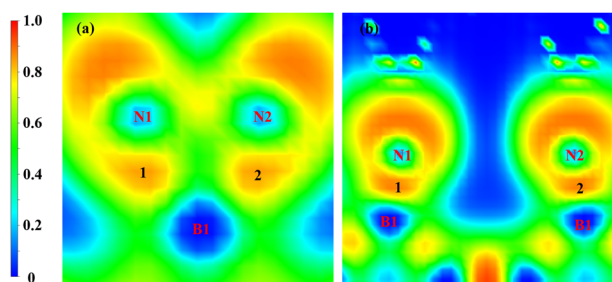
21620



### Gas-phase vibrational spectroscopy of the dysprosium monoxide molecule and its cation

Sascha Schaller, Sandy Gewinner, Wieland Schöllkopf, Gerard Meijer and André Fielicke\*

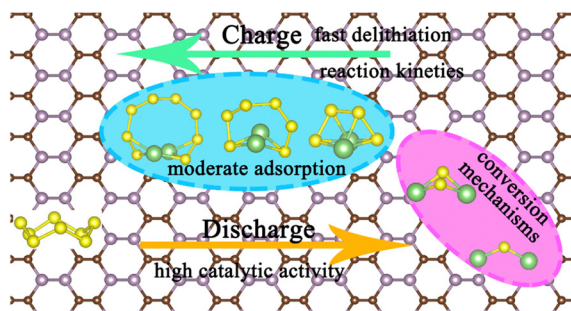
21628



### First-principles studies of gas molecule adsorption on a LaB<sub>6</sub>(100) surface

Rui Wang and Z. J. Ding\*

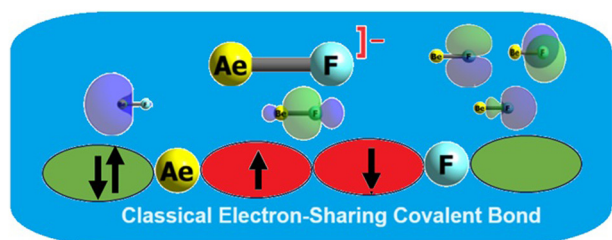
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### Two-dimensional phosphorus carbides (β-PC) as highly efficient metal-free electrocatalysts for lithium–sulfur batteries: a first-principles study

Junru Wang,\* Zhichao Liu, Yinchang Zhao, Zhenhong Dai, Juan Hua and Mingwen Zhao\*

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### Chemical bonding misnomer in AeF<sup>-</sup> (Ae = Be–Ca) anions

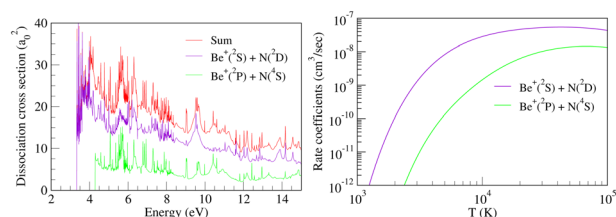
Ankur K. Guha



21659

### Theoretical study of a new molecular ion species $\text{BeN}^+$ : molecular states and cross sections for electronic excitation and dissociation

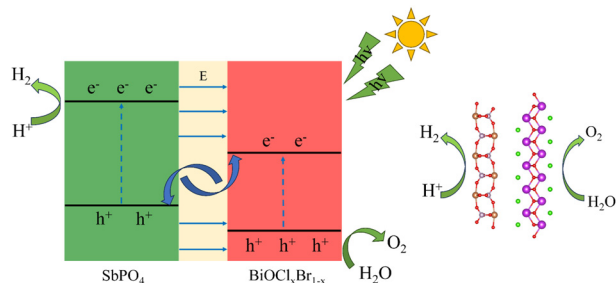
Kalyan Chakrabarti,\* Poonam Neogi and Gargi Nandi



21668

### Theoretical investigation of 2D/2D van der Waals $\text{SbPO}_4/\text{BiOCl}_x\text{Br}_{1-x}$ heterojunctions for photocatalytic water splitting

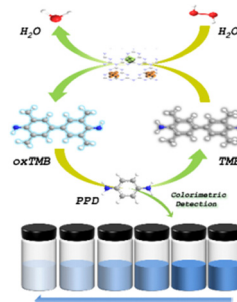
Zi Tao Zhu, Bo Wei Zhou, Zheng Dong Sun, Jia Xin Ma, Xiao Wang and Meng Zhang\*



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### Bimetal loaded graphitic carbon nitride with synergistic enhanced peroxidase-like activity for colorimetric detection of *p*-phenylenediamine

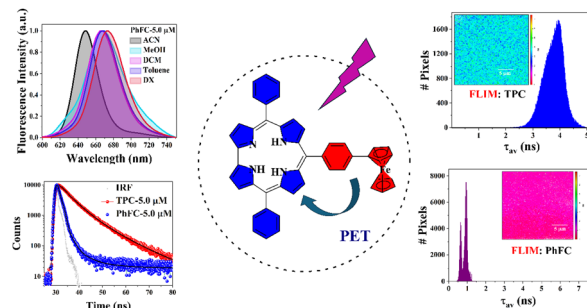
Jianshuai Mu, Mengjiao Ren, Ning Li, Tengyi Zhao, Zhong-Yi Liu, Jingwen Ma, Shulai Lei, Jiajun Wang,\* En-Cui Yang\* and Yan Wang\*



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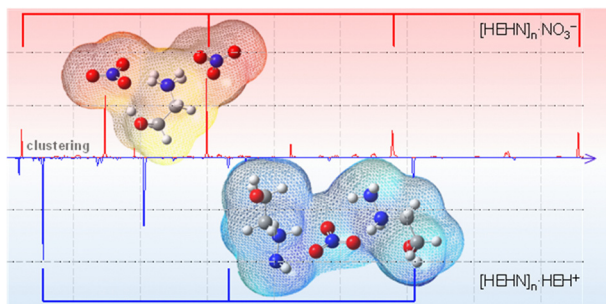
### Probing photoinduced electron transfer events in phenylferrocene–corrole dyad

Dineshbabu Takkella, Sudhanshu Sharma, Satyanarayana Samireddi\* and Krishna Gavvala\*



## RESEARCH PAPERS

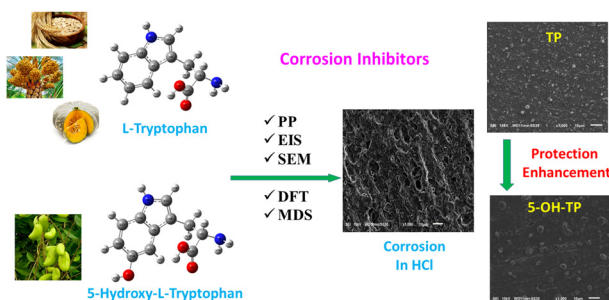
21697



### Dynamics and thermochemistry of the negatively charged clusters in a 2-hydroxyethylhydrazinium nitrate ionic liquid system

Wenjing Zhou, Jianbo Liu,\* Steven D. Chambreau and Ghanshyam L. Vaghjani

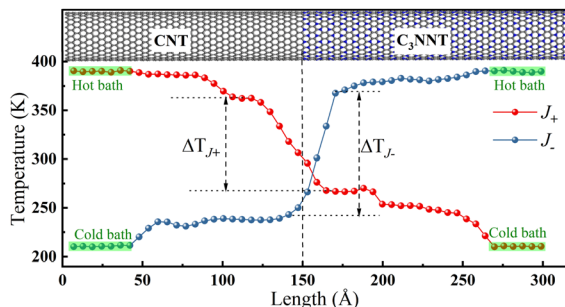
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### Corrosion inhibition ability of L-tryptophan and 5-hydroxy-L-tryptophan for mild steel: a combination of experimental and theoretical methods

Dinh Quy Huong,\* Nguyen Le My Linh, Le Quoc Thang and Duong Tuan Quang

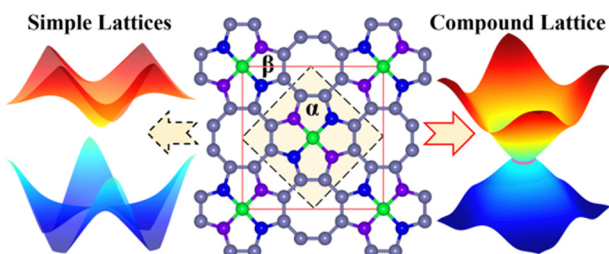
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### Prediction of high thermal rectification behavior in carbon/C<sub>3</sub>N heteronanotubes based on nonequilibrium molecular dynamics simulations

Zhibo Xing, Yingguang Liu,\* Ning Wu, Shuo Wang and Xutao Zhang

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### C-Me-graphene: an ideal two-dimensional nodal line semimetal with ultrahigh Young's modulus

Weixiang Kong,\* Xiaoliang Xiao, Juan Wei,\* Weiwei Xu, Bing Lv, Rui Wang and Xiaozhi Wu\*

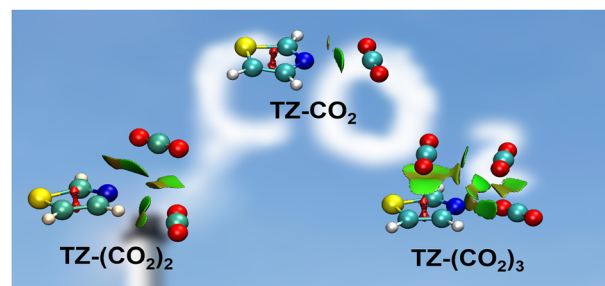


## RESEARCH PAPERS

21746

### Elucidating the non-covalent interactions in thiazole–carbon dioxide complexes through rotational spectroscopy and theoretical computations

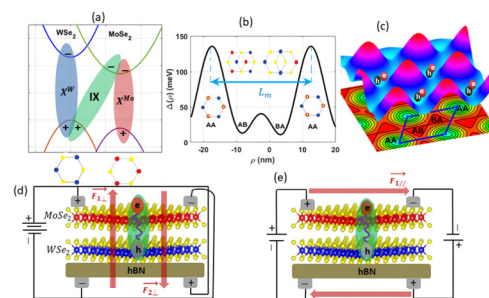
Liuting Wang, Tingting Yang, Zhen Wang and Gang Feng\*



21753

### Stark effect and orbital hybridization of moiré interlayer excitons in the MoSe<sub>2</sub>/WSe<sub>2</sub> heterobilayer

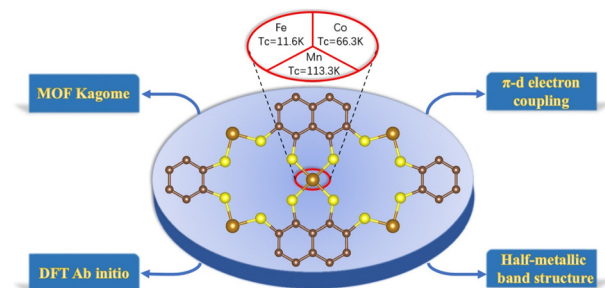
Housseem Eddine Hannachi\* and Sihem Jaziri



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### Effect of metal–ligand interactions on magnetic characteristics of two-dimensional Kagome structured perthiolated coronene (PTC) metal–organic frameworks (MOFs)

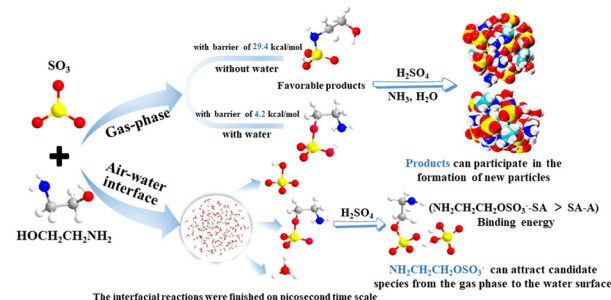
Zijie Fu, Yunfei Zhang, Minghao Jia, Shuo Zhang, Lixiu Guan, Dan Xing and Junguang Tao\*



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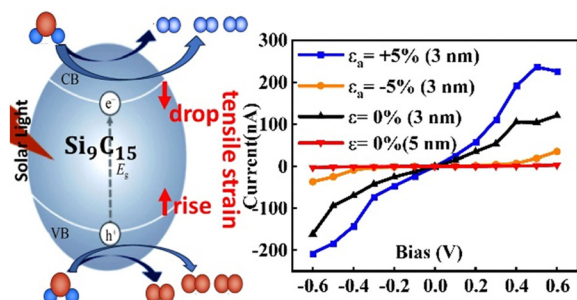
### The reaction mechanism of SO<sub>3</sub> with the multifunctional compound ethanolamine and its atmospheric implications

Rui Wang, Ruxue Mu, Zeyao Li, Yongqi Zhang, Jihuan Yang, Guanhua Wang and Tianlei Zhang\*



## RESEARCH PAPERS

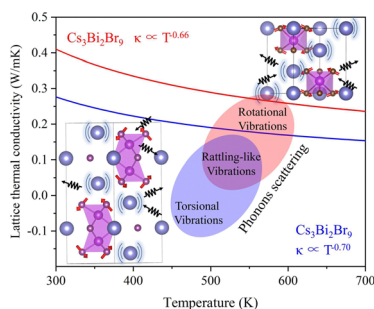
21789



Enhanced electron transport and optical properties of experimentally synthesized monolayer  $\text{Si}_9\text{C}_{15}$ : a comprehensive DFT study for nanoelectronics and photocatalytic applications

Yuehua Xu\* and Daqing Li

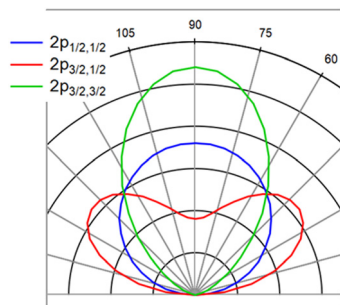
21801



Intrinsic ultralow lattice thermal conductivity in lead-free halide perovskites  $\text{Cs}_3\text{Bi}_2\text{X}_9$  ( $\text{X} = \text{Br}, \text{I}$ )

Jiang-Jiang Ma, Jing-Jing Zheng, Yuxi Chen, Qingyong Ren, Junfeng Zhang\* and Bao-Tian Wang\*

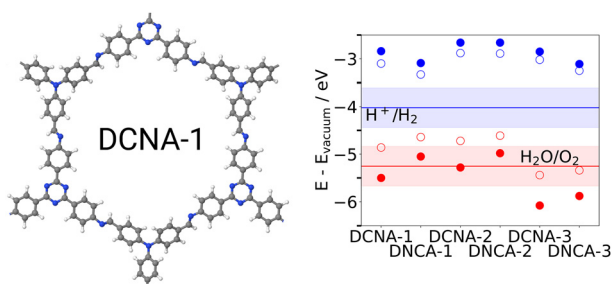
21810



Orientational anisotropy due to molecular field splitting in sulfur 2p photoemission from  $\text{CS}_2$  and  $\text{SF}_6$  – theoretical treatment and application to photoelectron recoil

Edwin Kukk,\* Johannes Niskanen, Oksana Travnikova, Marta Berholts, Kuno Kooser, Dawei Peng, Iyas Ismail, Maria Novella Piancastelli, Ralph Püttner, Uwe Hergerhahn and Marc Simon

21821



Water splitting at imine-linked covalent organic frameworks

Felizitas Gottwald, Christopher Penschke and Peter Saalfrank\*

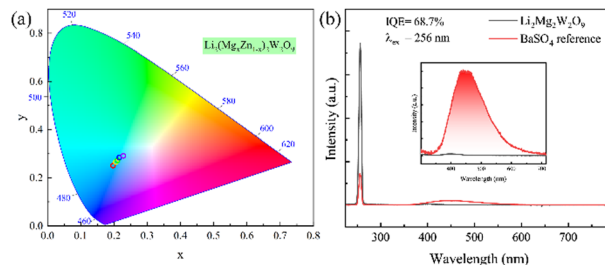


## RESEARCH PAPERS

21832

### Structural characterization of $\text{Li}_2(\text{Mg}_x\text{Zn}_{1-x})_2\text{W}_2\text{O}_9$ for bluish-white luminescence in rare earth-free tungstate phosphors

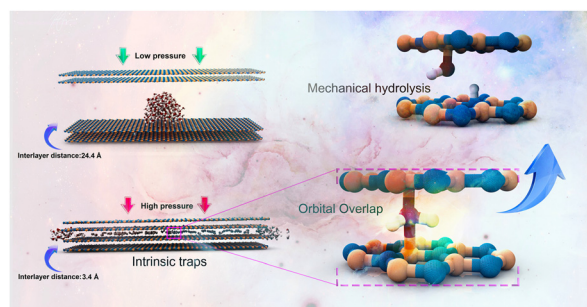
Jing Xie, Liang Li, Yue Zhong, Tao Su, Wenming Wang, Yan Pan, Xiantao Wei and Yong Li\*



21841

### Water molecules in boron nitride interlayer space: ice and hydrolysis in super confinement

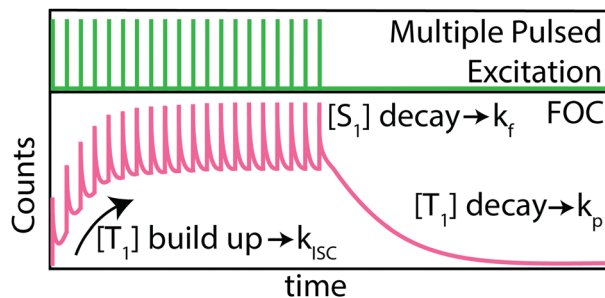
Amin Hosseini, Amir Masoud Yarahmadi, Shahab Azizi, Asghar Habibnejad Korayem\* and Rouzbeh Savary\*



21850

### Measuring the total photon economy of molecular species through fluorescent optical cycling

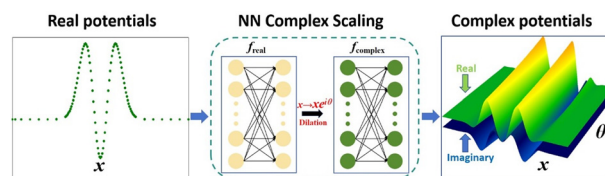
Anthony V. Sica, Ash Sueh Hua, Belle Coffey, Kierstyn P. Anderson, Lia A. Coffey, Benjamin T. Nguyen, Alexander M. Spokoyny and Justin R. Caram\*



21861

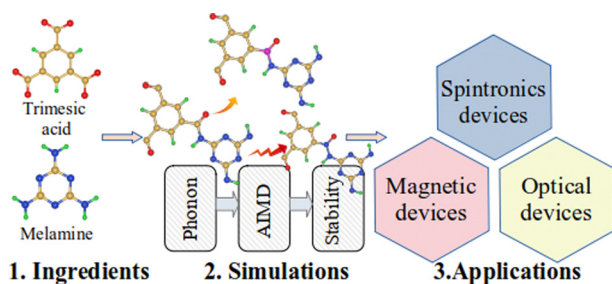
### Neural network potentials facilitating accurate complex scaling for molecular resonances: from a model to high dimensional realistic systems

Zhen Xu, Siting Hou, Zhimo Wang and Changjian Xie\*



## RESEARCH PAPERS

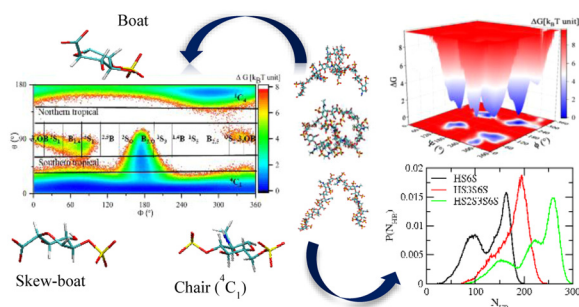
21874



### Modeling and tuning the electronic, mechanical and optical properties of a recently synthesized 2D polyaramid: a first principles study

Mukesh Singh, Surinder Pal Kaur and Brahmananda Chakraborty\*

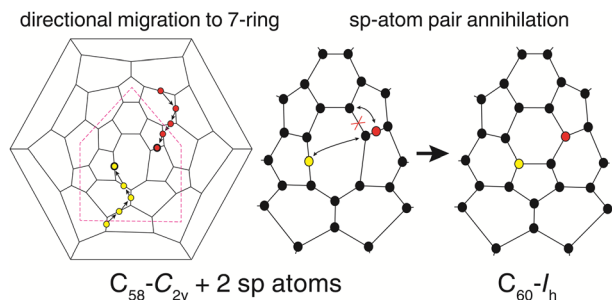
21888



### Conformational preferences of heparan sulfate to recognize the CXCL8 dimer in aqueous medium: degree of sulfation and hydrogen bonds

Shakuntala Dhurua and Madhurima Jana\*

21905



### Formation of the icosahedral $C_{60}$ fullerene via migration of single sp atoms and annihilation of sp-atom pairs

Alexander S. Sinitsa,\* Yulia G. Polynskaya, Nikita A. Matsokin, Yegor M. Kedalo, Andrey A. Knizhnik and Andrey M. Popov

## CORRECTION

21912

### Correction: Nonequilibrium thermodynamic model of thermoelectricity and thermodiffusion in semiconductors

Semen N. Semenov\* and Martin E. Schimpf

