

## IN THIS ISSUE

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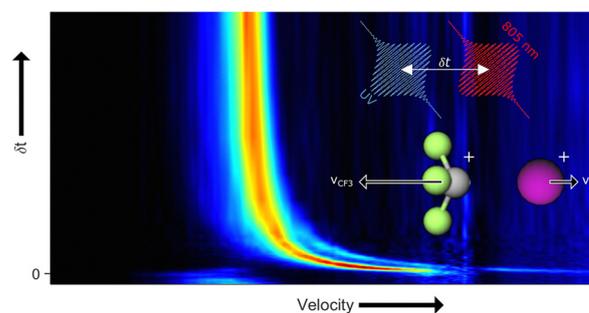
See Michael N. R. Ashfold *et al.*, pp. 16672–16698. Image reproduced by permission of Stuart Crane from *Phys. Chem. Chem. Phys.*, 2023, 25, 16672.

## PERSPECTIVE

16672

### Molecular photodissociation dynamics revealed by Coulomb explosion imaging

Stuart W. Crane, Jason W. L. Lee, Michael N. R. Ashfold\* and Daniel Rolles

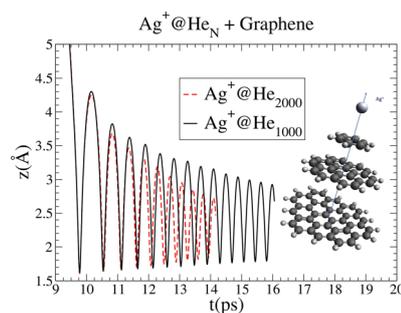


## COMMUNICATIONS

16699

### Superfluid helium droplet-mediated surface-deposition of neutral and charged silver atomic species

Berta Fernández, Martí Pi and María Pilar de Lara-Castells\*



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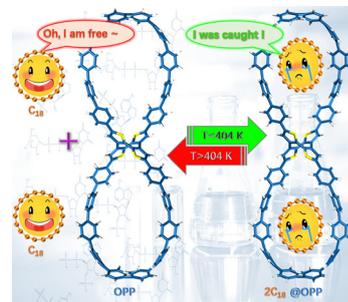


## COMMUNICATIONS

16707

## Molecular assembly with a figure-of-eight nano hoop as a strategy for the collection and stabilization of cyclo[18]carbon

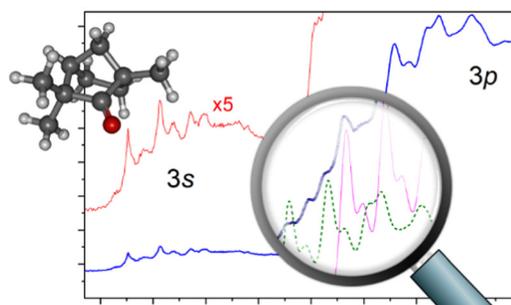
Zeyu Liu,\* Xia Wang, Tian Lu,\* Jiaojiao Wang, Xiufen Yan, Yang Wu and Jingbo Xu



16712

## The Rydberg 3p multiplet structure of the fenchone C band absorption

Ivan Powis\* and Dharendra P. Singh

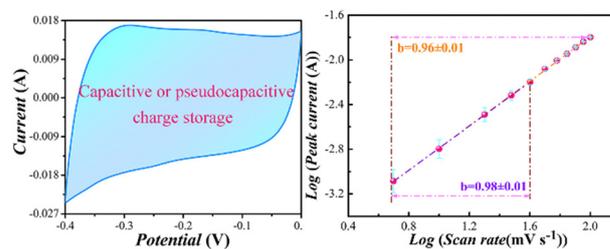


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## What about electrochemical behaviors for aurivillius-phase bismuth tungstate? Capacitive or pseudocapacitive

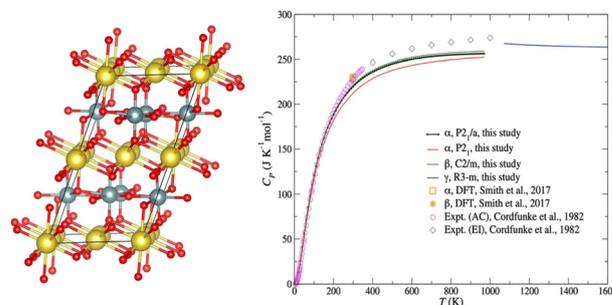
Jian-Fei Gao, Jing-Feng Hou and Ling-Bin Kong\*



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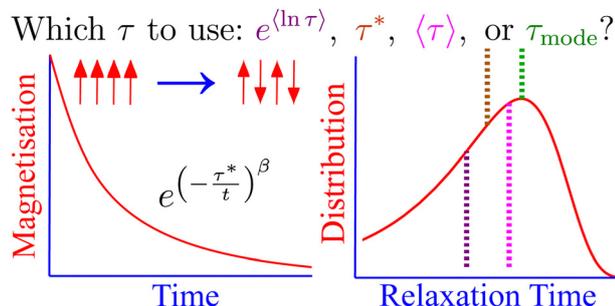
Polymorphism and phase transitions in Na<sub>2</sub>U<sub>2</sub>O<sub>7</sub> from density functional perturbation theory

Philippe F. Weck,\* Carlos F. Jové-Colón and Eunja Kim



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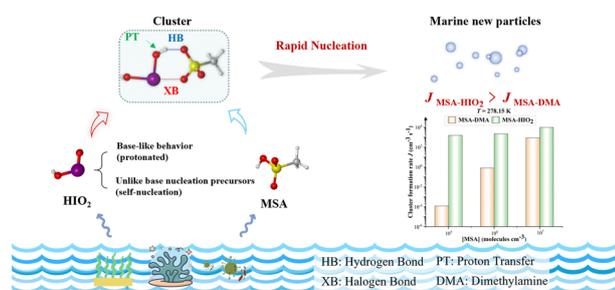
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### Characterisation of magnetic relaxation on extremely long timescales

William J. A. Blackmore, Gemma K. Gransbury, Peter Evans, Jon G. C. Kragoskow, David P. Mills\* and Nicholas F. Chilton\*

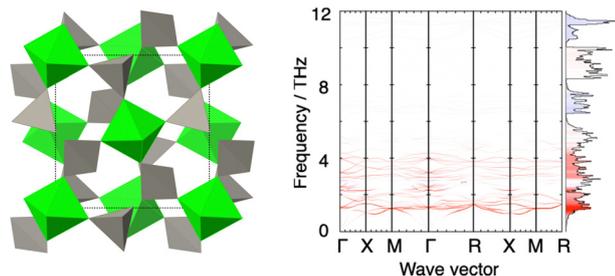
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### Methanesulfonic acid and iodosic acid nucleation: a novel mechanism for marine aerosols

Nan Wu, An Ning,\* Ling Liu, Haotian Zu, Danli Liang and Xiuhui Zhang\*

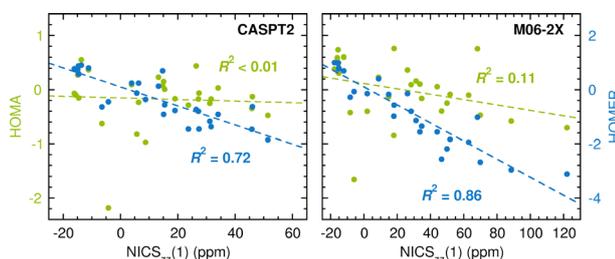
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### Phonon mechanism for the negative thermal expansion of zirconium tungstate, $\text{ZrW}_2\text{O}_8$

Leila H. N. Rimmer, Keith Refson and Martin T. Dove\*

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### HOMER: a reparameterization of the harmonic oscillator model of aromaticity (HOMA) for excited states

Enrique M. Arpa\* and Bo Durbej\*

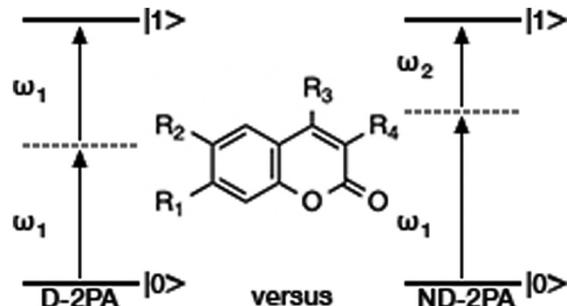


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**Degenerate and non-degenerate two-photon absorption of coumarin dyes**

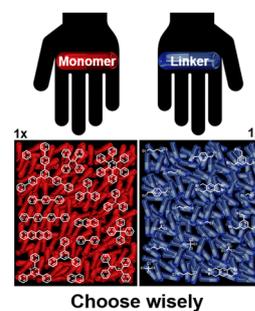
Ismael A. Elayan and Alex Brown\*



16781

**Rationalizing the formation of porosity in mechanochemically-synthesized polymers**

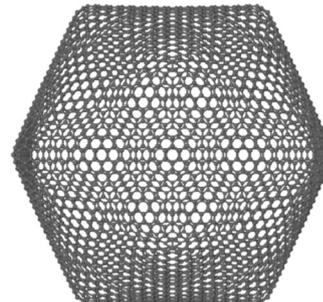
Annika Krusenbaum, Steffi Krause Hinojosa, Sven Fabig, Valentin Becker, Sven Grätz and Lars Borchardt\*



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**The largest fullerene**

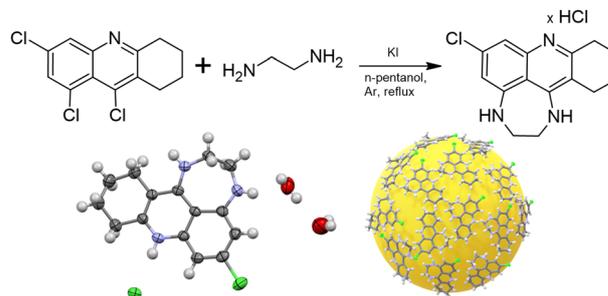
Michael Gatchell, Henning Zettergren and Klavs Hansen\*



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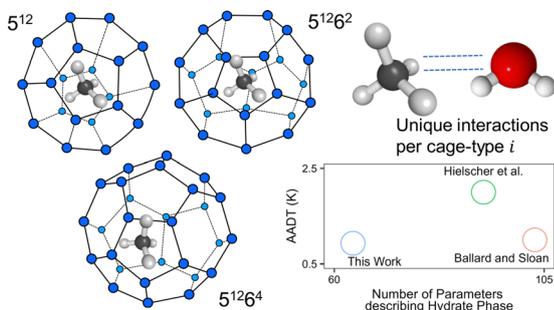
**A tetrahydroacridine derivative and its conjugate with gold nanoparticles: promising agents for the treatment of Alzheimer's disease**

Ilona Mojzych, Anna Zawadzka, Katarzyna Kaczyńska, Piotr Wojciechowski, Dominika Zajac, Maciej Chotkowski, Katarzyna Wiktorska, Jan K. Maurin and Maciej Mazur\*



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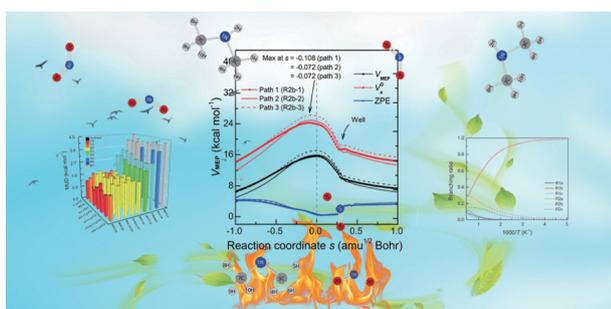
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### A cage-specific hydrate equilibrium model for robust predictions of industrially-relevant mixtures

David J. Zhu, Bruce W. E. Norris, Zachary M. Aman\* and Eric F. May\*

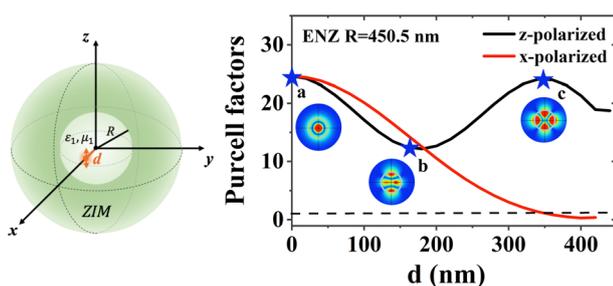
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### Advanced kinetic calculations with multi-path variational transition state theory for reactions between dimethylamine and nitrogen dioxide in atmospheric and combustion temperature ranges

Yanlei Shang

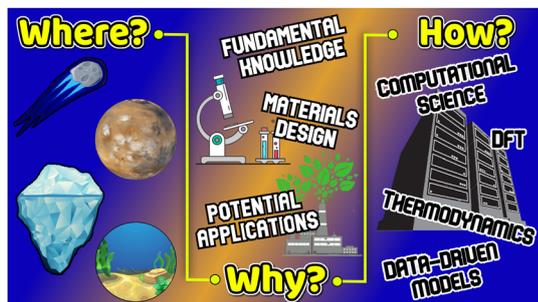
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### Inhibition and enhancement of the spontaneous emission in spherical cavities surrounded by zero-index-materials

Yun Ma, Qi Liu, Lingxiao Shan, Xinchun Zhang, Yali Jia, Qihuang Gong and Ying Gu\*

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### Computational investigations of stable multiple-cage-occupancy He clathrate-like hydrostructures

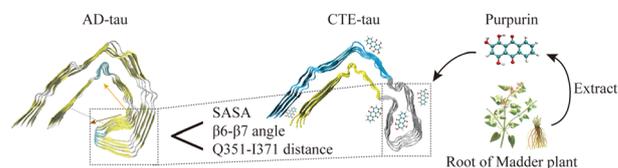
Raquel Yanes-Rodriguez and Rita Prosimiti\*



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### Destabilization mechanism of R3–R4 tau protofilament by purpurin: a molecular dynamics study

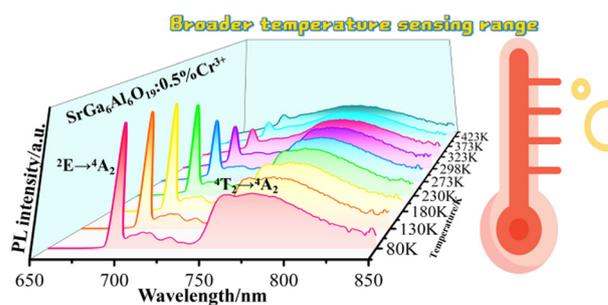
Jiaqian Wan, Yu Zou, Ruiqing Sun, Zhengdong Xu, Jiaying Tang, Yehong Gong, Guanghong Wei\* and Qingwen Zhang\*



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### Extending the optical temperature sensing range of Cr<sup>3+</sup> by synchronously tuning <sup>2</sup>E and <sup>4</sup>T<sub>2</sub> emission

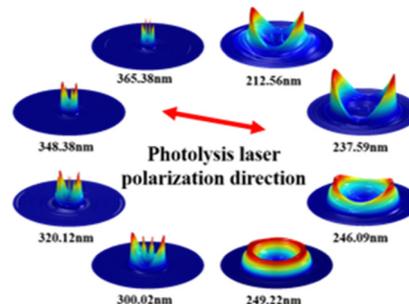
Jiaqi Ou, Shuangqiang Fang,\* Qiangqiang Zhu, Yue Zhai, Hong Zhang and Le Wang\*



16872

### Slice imaging study of NO<sub>2</sub> photodissociation via the 1<sup>2</sup>B<sub>2</sub> and 2<sup>2</sup>B<sub>2</sub> states: the NO(X<sup>2</sup>Π) + O(<sup>3</sup>P<sub>J</sub>) product channel

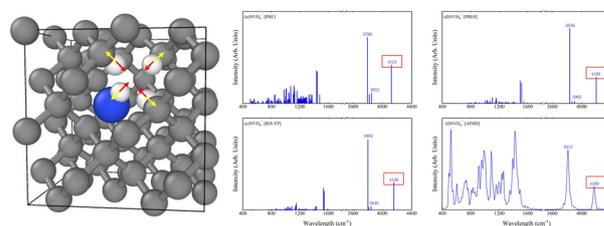
Zhaoxue Zhang, Shuaikang Yang, Zhenxing Li,\* Yao Chang, Zijie Luo, Yarui Zhao, Shengrui Yu,\* Kaijun Yuan\* and Xueming Yang



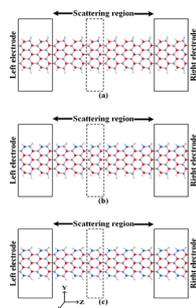
16881

### The search for a band of a defect predicted above 4000 cm<sup>-1</sup> in diamond through infrared vibrational spectra: a quantum mechanical investigation

Yanyan Zhang, Libin Zhang, Dongliang Zhang, Yichen Li, Sheng Liu, Bo Yang\* and Zhiyin Gan\*



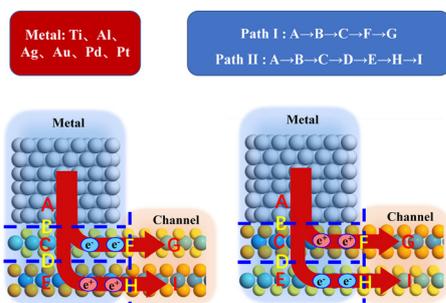
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### Nitrogen-doped zinc oxide nanoribbons for potential resonant tunneling diode applications

M. Sankush Krishna,\* Sangeeta Singh and Brajesh Kumar Kaushik

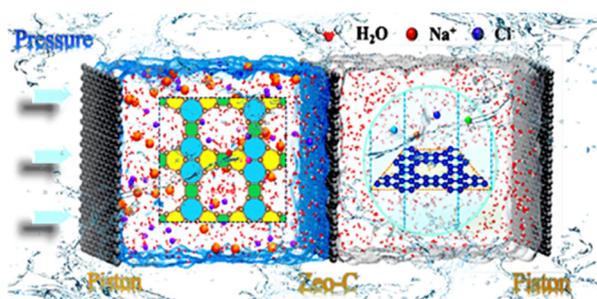
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### Dual transmission channels at metal–MoS<sub>2</sub>/WSe<sub>2</sub> hetero-bilayer interfaces

Dongqing Zou, Wenkai Zhao,\* Yuqing Xu, Xiaoteng Li, Yuliang Liu and Chuanlu Yang\*

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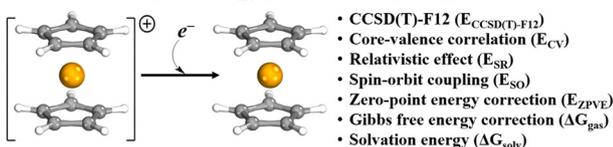


### Computational simulation-driven discovery of novel zeolite-like carbon materials as seawater desalination membranes

Kun Meng, Xiuhan Li, Yutao Niu, Changhong Zhang, Xiaohua Yu, Ju Rong, Hongying Hou\* and Hui Chen\*

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Absolute reduction potential ( $E_{\text{abs}}^{\ominus}$ ) predictions for  $\text{Cp}_2\text{M}^{\oplus}/\text{Cp}_2\text{M}$  ( $\text{M}=\text{Fe}, \text{Co}$  and  $\text{Ni}$ )



### Ferrocene/ferrocenium, cobaltocene/cobaltocenium and nickelocene/nickelocenium: from gas phase ionization energy to one-electron reduction potential in solvated medium

Hongyan Zhao, Yi Pan and Kai-Chung Lau\*

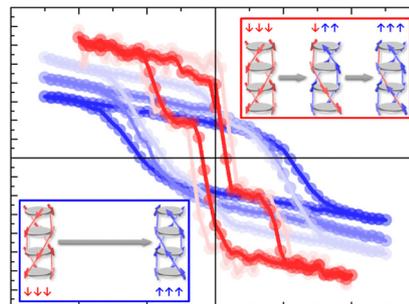


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### Ferro- and ferrielectricity and negative piezoelectricity in thioamide-based supramolecular organic discotics

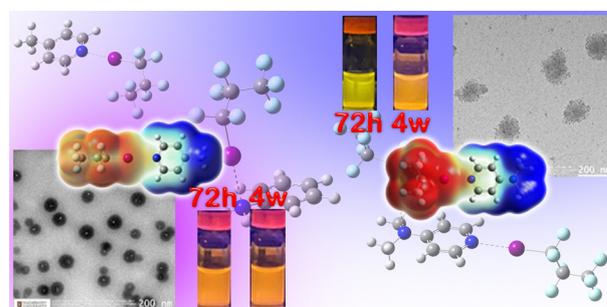
Indre Urbanaviciute, Miguel Garcia-Iglesias, Andrey Gorbunov, E. W. Meijer and Martijn Kemerink\*



16938

### Fluorescent nano-sized aggregates of halogen bonded complexes formed using perfluoropropyl iodides: a systematic comparison between two isomeric halogen bond acceptors, aniline and 4-methyl pyridine

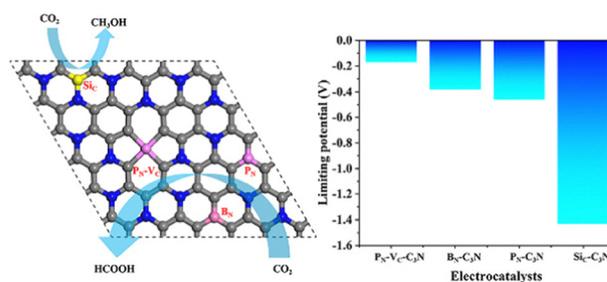
Haiyan Fan, Lazzat Nurtay, Nurgul Daniyeva and Enrico Benassi\*



16952

### Unravelling the adsorption and electroreduction performance of CO<sub>2</sub> and N<sub>2</sub> over defective and B, P, Si-doped C<sub>3</sub>Ns: a DFT study

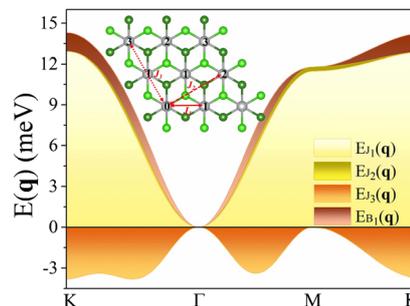
Dandan Wang, Xueting Liu, Huiru Yang, Ziang Zhao, Yucheng Liu, Xin Qu, Lihua Yang, Ming Feng\* and Zaicheng Sun\*



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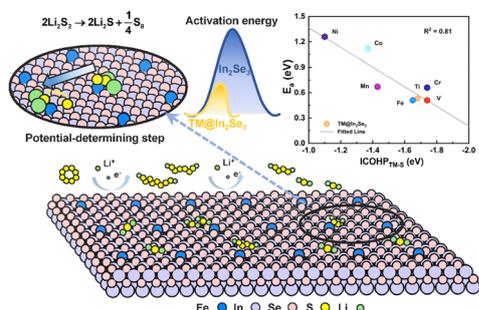
### Same effect of biquadratic exchange interaction and Heisenberg linear interaction in a spin spiral

Lingzi Jiang, Can Huang, Bingjie Liu, Yanfei Pan, Jiyu Fan, Daning Shi,\* Chunlan Ma\* and Yan Zhu\*



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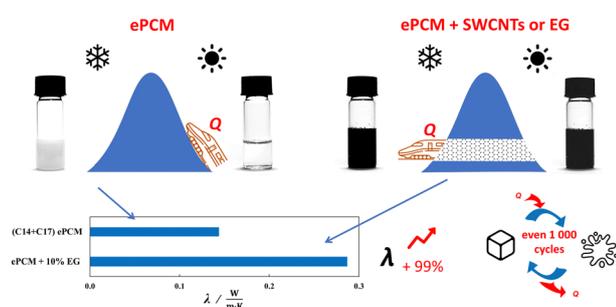
16968



### Identification of linear scaling relationships in polysulfide conversion on $\alpha$ - $\text{In}_2\text{Se}_3$ -supported single-atom catalysts

Hui Wang, Lin Zou, Min Li and Long Zhang\*

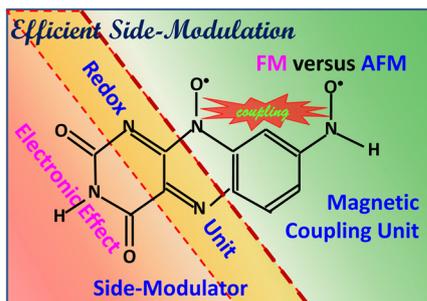
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### Alkane-based eutectic phase change materials doped with carbon nanomaterials

Mikołaj Więckowski,\* Marek Królikowski, Łukasz Scheller and Marzena Dzida

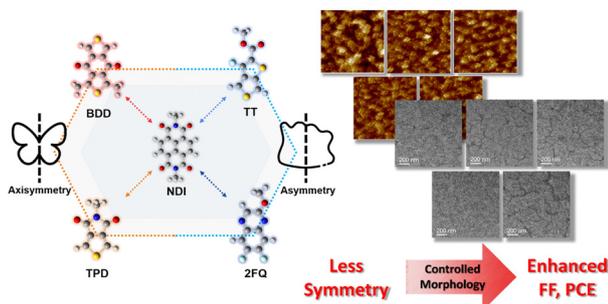
16991



### Magnetic coupling modulation in *meta*-nitroxide-functionalized isoalloxazine magnets with redox-active units as efficient side-modulators

Rabia Malik and Yuxiang Bu\*

17001



### Naphthalene diimide-based random terpolymers with axisymmetric and asymmetric electron acceptors for controllable morphology and enhanced fill factors in all-polymer solar cells

Geunhyung Park, Yongjoon Cho, Seunglok Lee, Seungju Kim, Kyu Cheol Lee\* and Changduk Yang\*

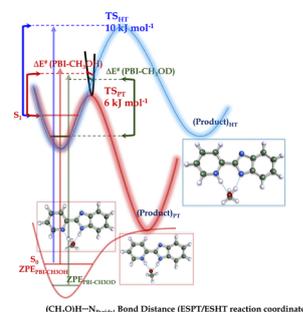


## RESEARCH PAPERS

17010

### A combined spectroscopic and computational investigation on the solvent-to-chromophore excited-state proton transfer in the 2,2'-pyridylbenzimidazole–methanol complex

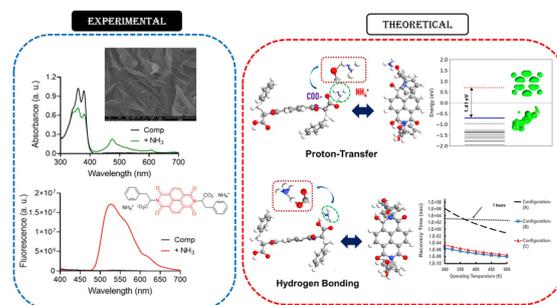
Ramesh Jarupula, Saurabh Khodia, Muhammed Shabeeb and Surajit Maity\*



17021

### Site-specific ammonia adsorption and transduction on a naphthalimide derivative molecule – a complementary analysis involving *ab initio* calculation and experimental verification

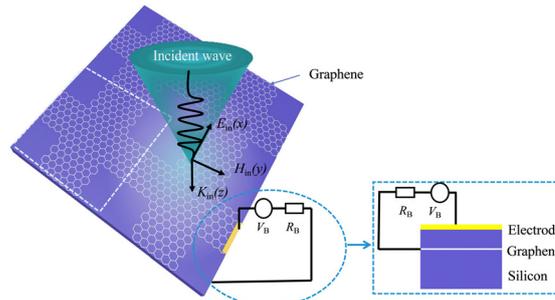
Aditya Tiwari, Rikitha S. Fernandes, Nilanjan Dey\* and Sayan Kanungo\*



17034

### Polarization-independent plasmon-induced transparency and slow light effects in a fully continuous symmetric cross-shaped monolayer graphene structure

Can Wan, Cuixiu Xiong,\* Meng Tan, Chengya Wei, Jie Wang and Saiwen Zhang



17043

### GO nanosheets decorated with SnS nanoparticles: excellent photocatalytic performance under visible-light irradiation

Elham Kharatzadeh\* and Marzieh Khademalrasool\*

