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Cover

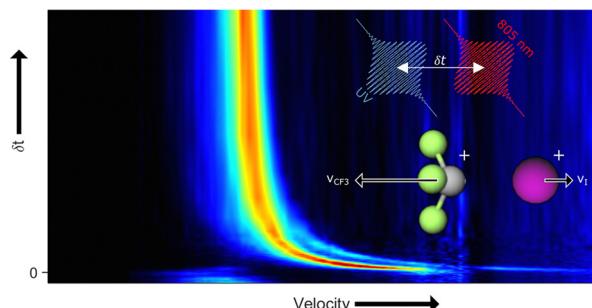
See Michael N. R. Ashfold et al., pp. 16672–16698.
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PERSPECTIVE

16672

Molecular photodissociation dynamics revealed by Coulomb explosion imaging

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

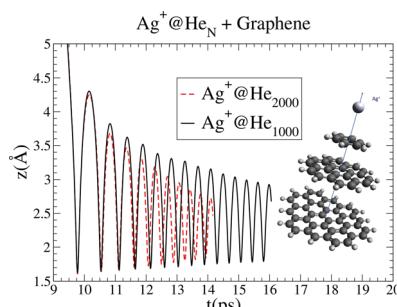


COMMUNICATIONS

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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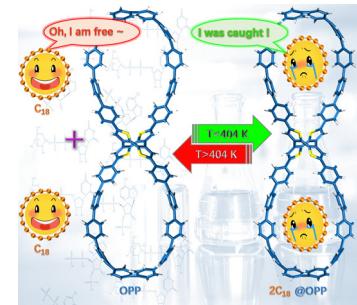


COMMUNICATIONS

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

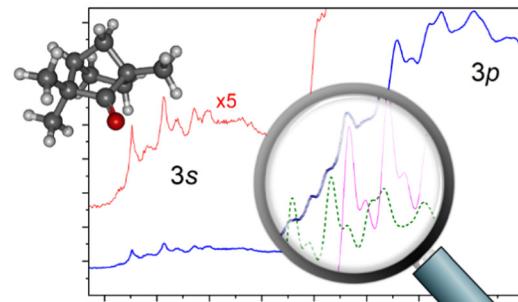
Zeyu Liu,* Xia Wang, Tian Lu,* Jiaojiao Wang, Xiufen Yan, Yang Wu and Jingbo Xu



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

Ivan Powis* and Dhirendra P. Singh

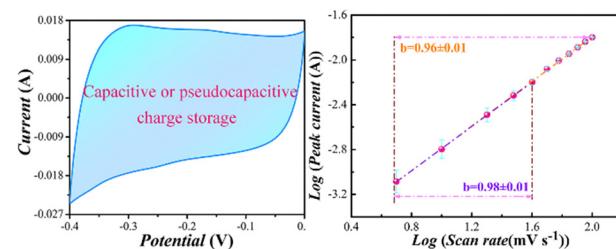


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What about electrochemical behaviors for aurivillius-phase bismuth tungstate? Capacitive or pseudocapacitive

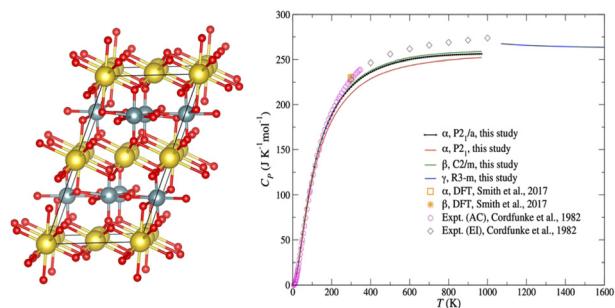
Jian-Fei Gao, Jing-Feng Hou and Ling-Bin Kong*



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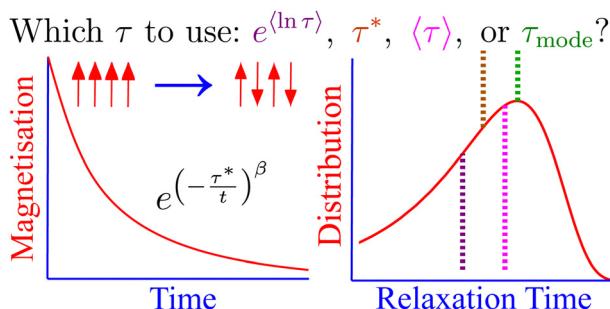
Polymorphism and phase transitions in $\text{Na}_2\text{U}_2\text{O}_7$ from density functional perturbation theory

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



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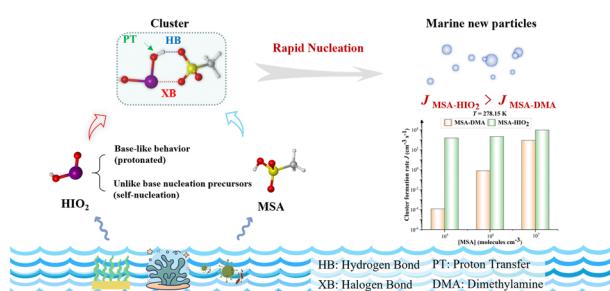
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Characterisation of magnetic relaxation on extremely long timescales

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

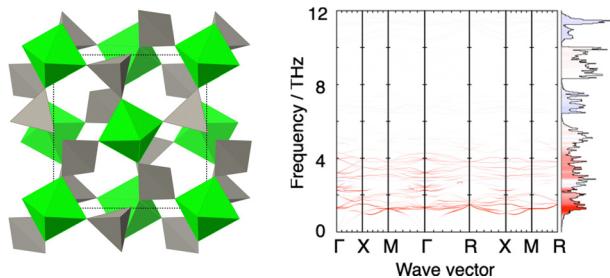
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Methanesulfonic acid and iodous acid nucleation: a novel mechanism for marine aerosols

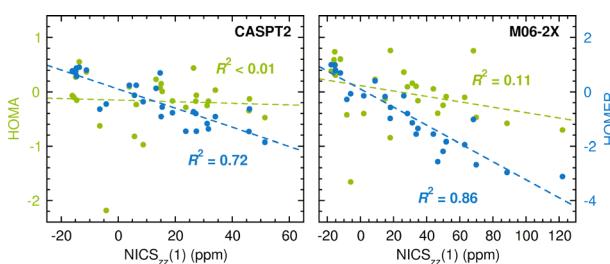
Nan Wu, An Ning,* Ling Liu, Haotian Zu, Danli Liang and Xiuwei Zhang*

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Phonon mechanism for the negative thermal expansion of zirconium tungstate, ZrW_2O_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 Durbeej*

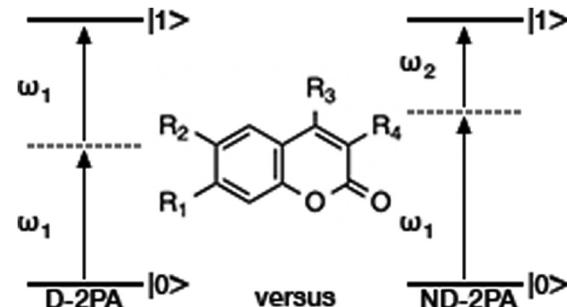


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Degenerate and non-degenerate two-photon absorption of coumarin dyes

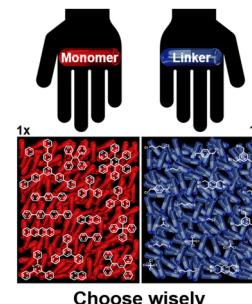
Ismael A. Elayan and Alex Brown*



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Rationalizing the formation of porosity in mechanochemically-synthesized polymers

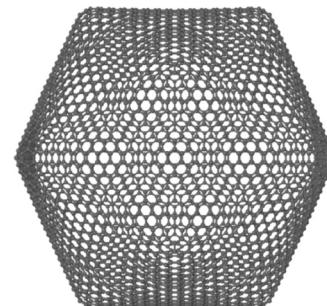
Annika Krusenbaum, Steffi Krause Hinojosa, Sven Fabig, Valentin Becker, Sven Grätz and Lars Borchardt*



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The largest fullerene

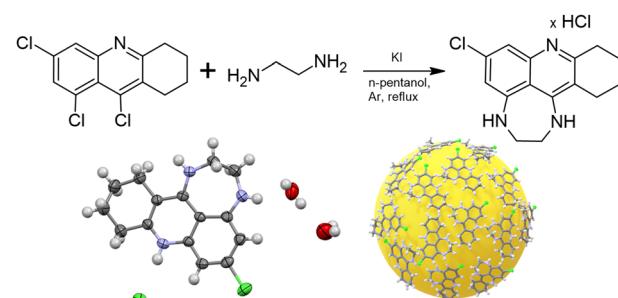
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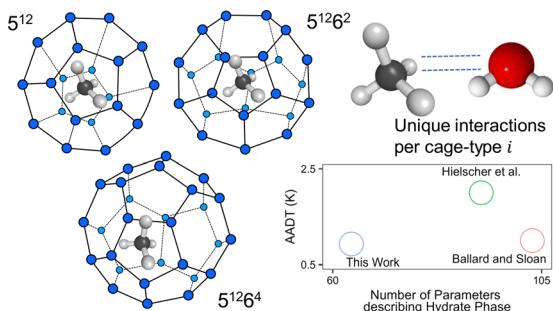
A tetrahydroacridine derivative and its conjugate with gold nanoparticles: promising agents for the treatment of Alzheimer's disease

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



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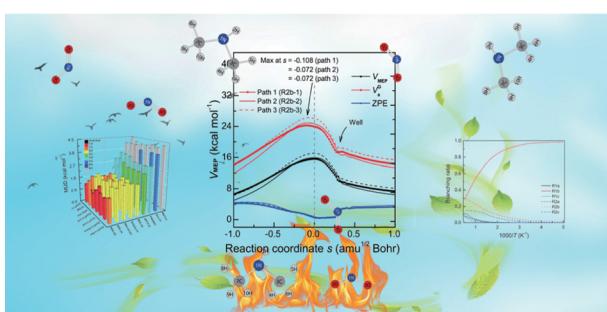
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A cage-specific hydrate equilibrium model for robust predictions of industrially-relevant mixtures

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

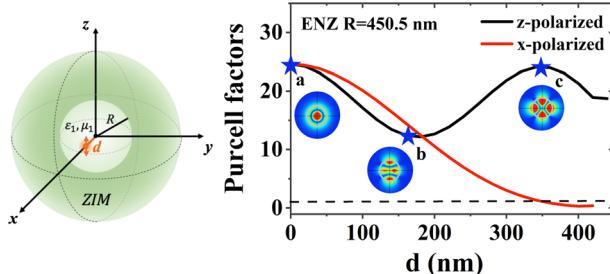
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Yanlei Shang

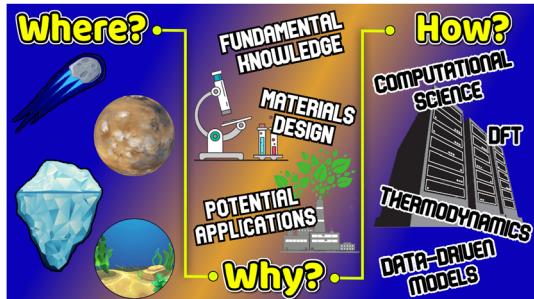
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Yun Ma, Qi Liu, Lingxiao Shan, Xinchen Zhang, Yali Jia, Qihuang Gong and Ying Gu*

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

Raquel Yanes-Rodríguez and Rita Prosmiti*

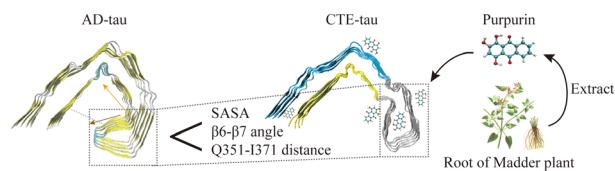


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Destabilization mechanism of R3–R4 tau protofilament by purpurin: a molecular dynamics study

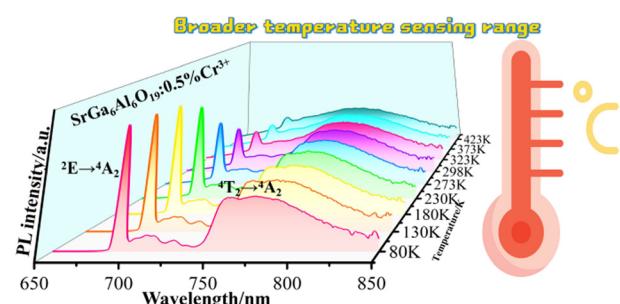
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Extending the optical temperature sensing range of Cr³⁺ by synchronously tuning ²E and ⁴T₂ emission

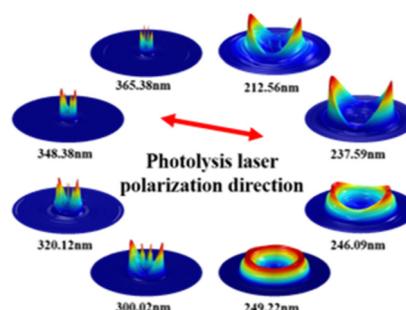
Jiaqi Ou, Shuangqiang Fang,* Qiangqiang Zhu, Yue Zhai, Hong Zhang and Le Wang*



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Slice imaging study of NO₂ photodissociation via the 1²B₂ and 2²B₂ states: the NO(X²Π) + O(³P_J) product channel

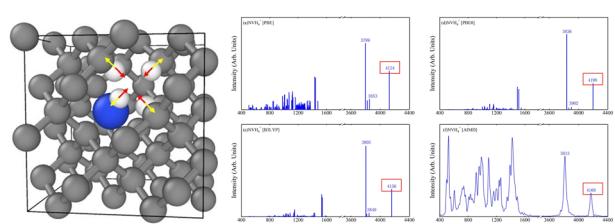
Zhaoxue Zhang, Shuaikang Yang, Zhenxing Li,* Yao Chang, Zijie Luo, Yarui Zhao, Shengrui Yu,* Kaijun Yuan* and Xueming Yang



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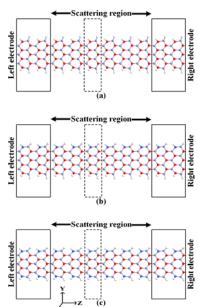
The search for a band of a defect predicted above 4000 cm⁻¹ in diamond through infrared vibrational spectra: a quantum mechanical investigation

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



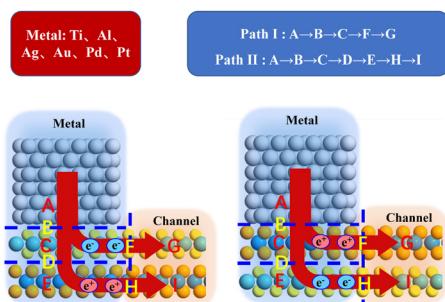
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Nitrogen-doped zinc oxide nanoribbons for potential resonant tunneling diode applications

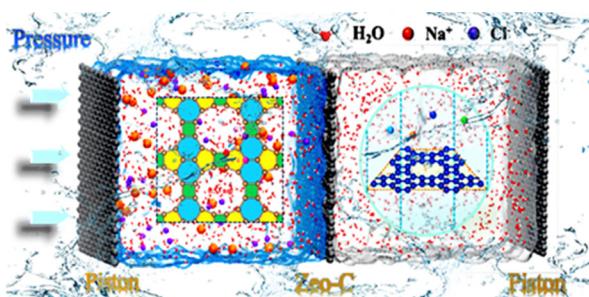
 M. Sankush Krishna,* Sangeeta Singh and
 Brajesh Kumar Kaushik

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Dual transmission channels at metal–MoS₂/WSe₂ hetero-bilayer interfaces

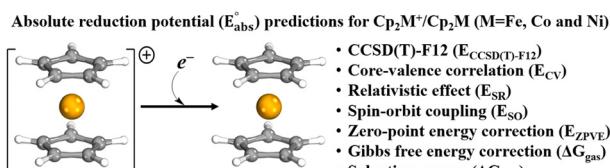
Dongqing Zou, Wenkai Zhao,* Yuqing Xu, Xiaoteng Li, Yuliang Liu and Chuanlu Yang*

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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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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*

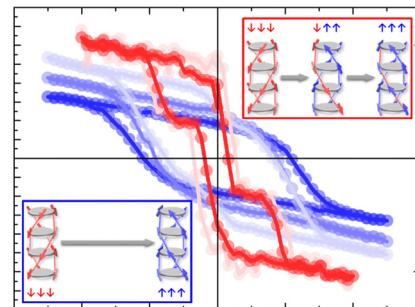


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Ferro- and ferrielectricity and negative piezoelectricity in thioamide-based supramolecular organic discotics

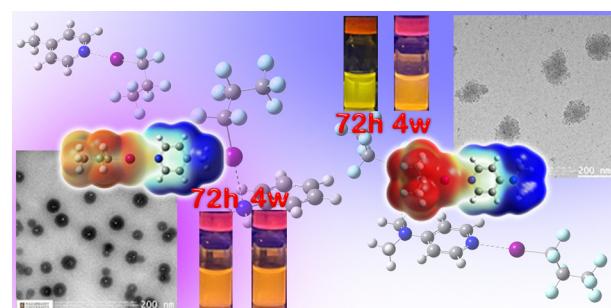
Indre Urbanaviciute, Miguel Garcia-Iglesias, Andrey Gorbunov, E. W. Meijer and Martijn Kemerink*



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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

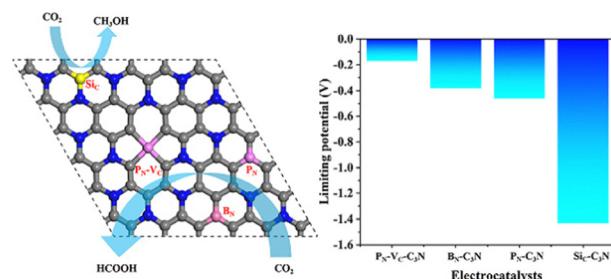
Haiyan Fan, Lazzat Nurtay, Nurgul Daniyeva and Enrico Benassi*



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Unravelling the adsorption and electroreduction performance of CO₂ and N₂ over defective and B, P, Si-doped C₃Ns: a DFT study

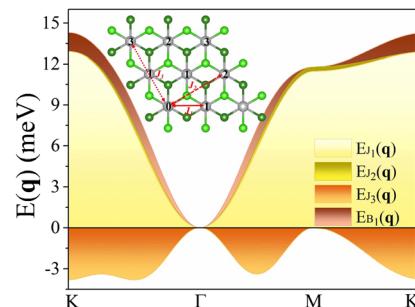
Dandan Wang, Xuetong Liu, Huiru Yang, Ziang Zhao, Yucheng Liu, Xin Qu, Lihua Yang, Ming Feng* and Zaicheng Sun*



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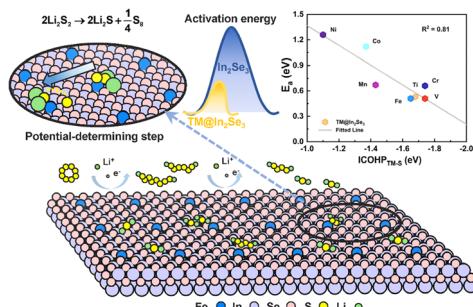
Same effect of biquadratic exchange interaction and Heisenberg linear interaction in a spin spiral

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



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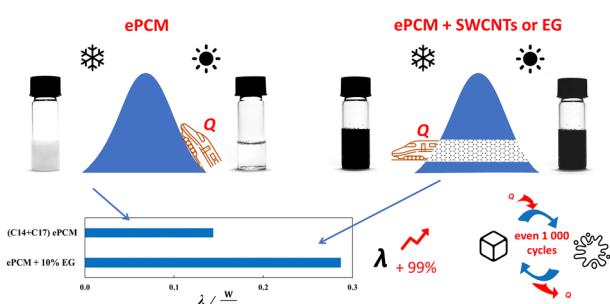
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Identification of linear scaling relationships in polysulfide conversion on α -In₂Se₃-supported single-atom catalysts

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

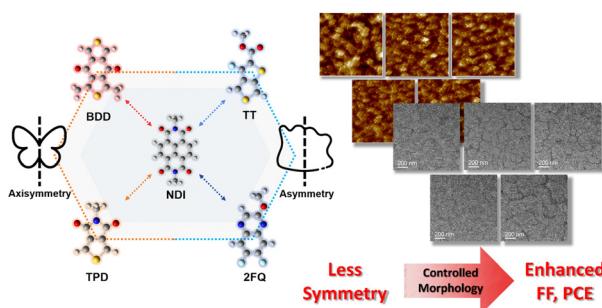
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Magnetic coupling modulation in meta-nitroxide-functionalized isoalloxazine magnets with redox-active units as efficient side-modulators

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*

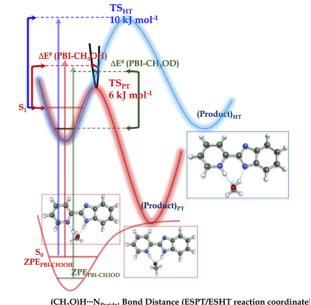


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A combined spectroscopic and computational investigation on the solvent-to-chromophore excited-state proton transfer in the 2,2'-pyridylbenzimidazole–methanol complex

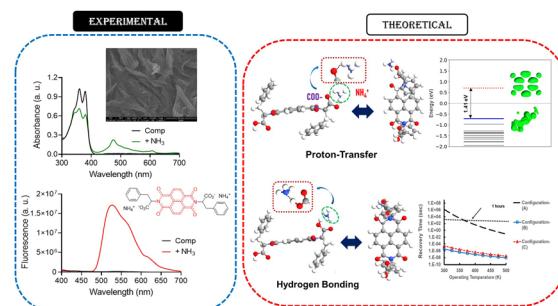
Ramesh Jarupula, Saurabh Khodia, Muhammed Shabeeb and Surajit Maity*



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

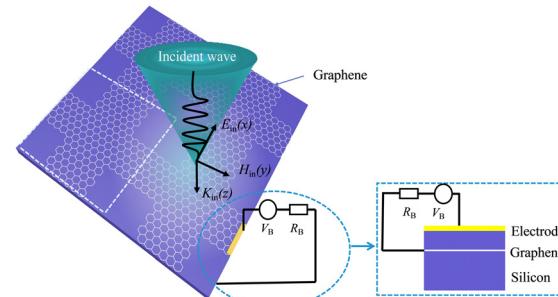
Aditya Tiwari, Rikitha S. Fernandes, Nilanjan Dey* and Sayan Kanungo*



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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



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

Elham Kharatzadeh* and Marzieh Khademalrasool*

