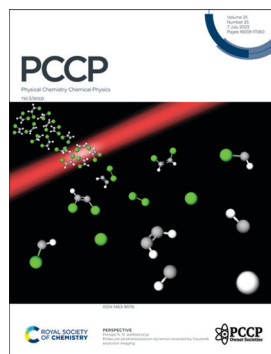


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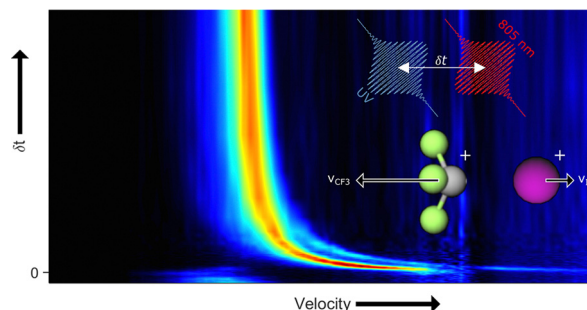
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PERSPECTIVE

16672

Molecular photodissociation dynamics revealed by Coulomb explosion imaging

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

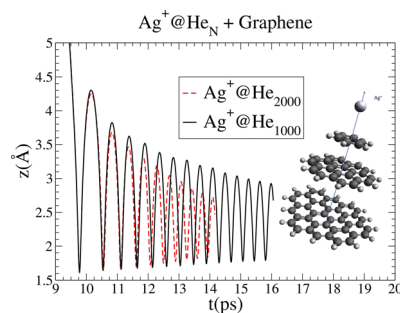


COMMUNICATIONS

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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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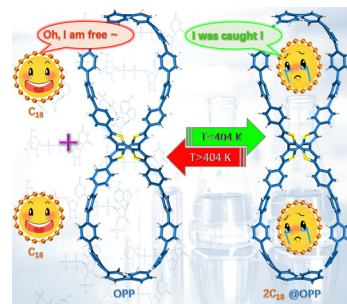


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Molecular assembly with a figure-of-eight nanohoop as a strategy for the collection and stabilization of cyclo[18]carbon

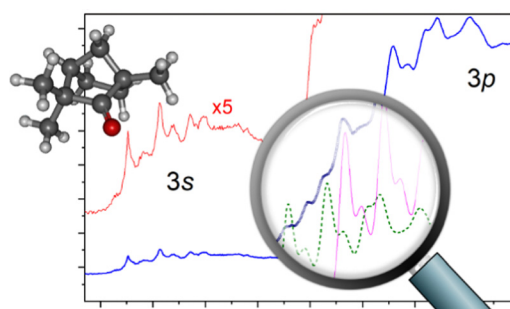
Zeyu Liu,* Xia Wang, Tian Lu,* Jiaojiao Wang, Xiufen Yan, Yang Wu and Jingbo Xu



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

Ivan Powis* and Dharendra P. Singh

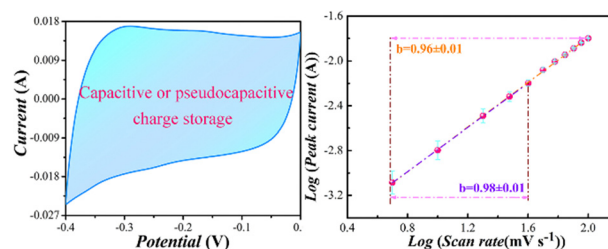


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What about electrochemical behaviors for aurivillius-phase bismuth tungstate? Capacitive or pseudocapacitive

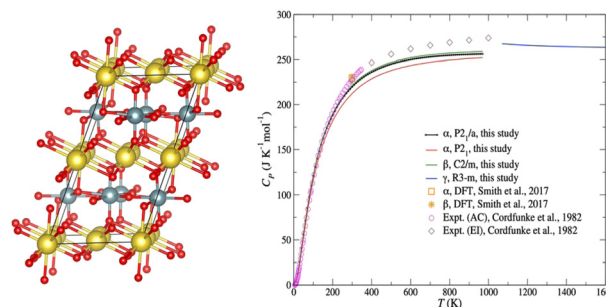
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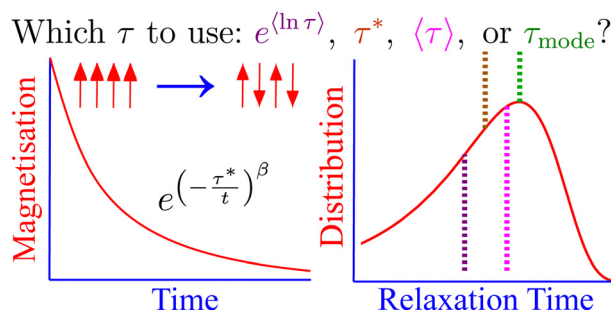
Polymorphism and phase transitions in Na₂U₂O₇ from density functional perturbation theory

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



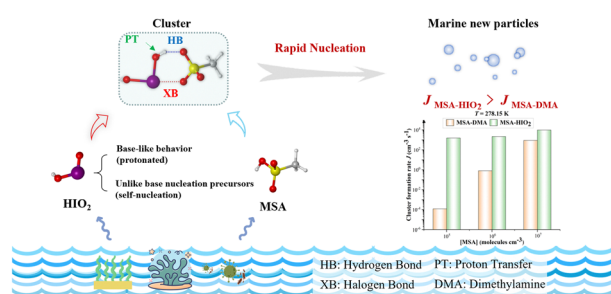
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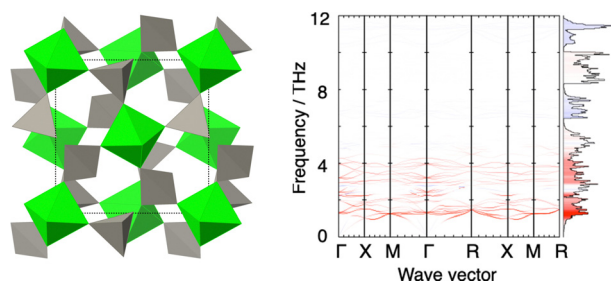
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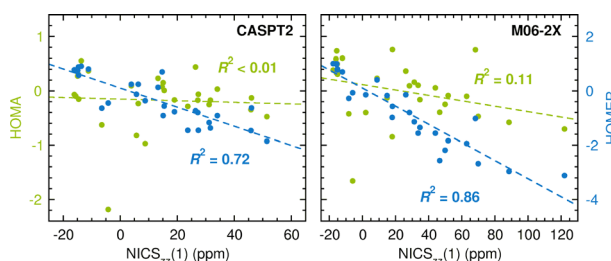
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**HOMER: a reparameterization of the harmonic oscillator model of aromaticity (HOMA) for excited states**

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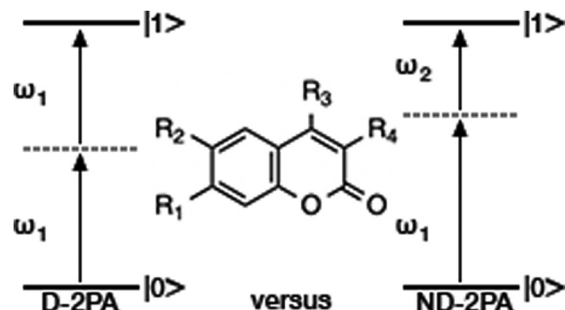


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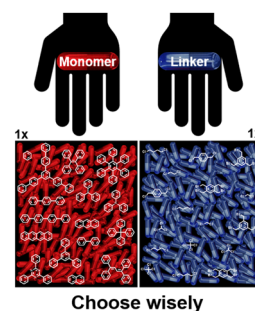
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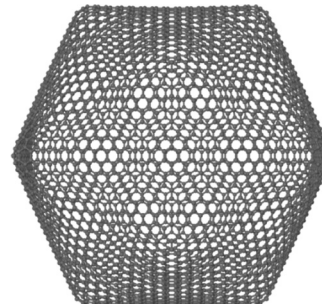
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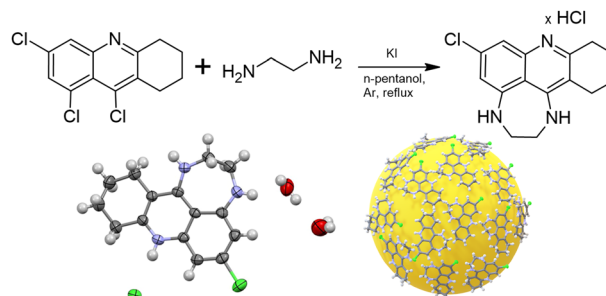
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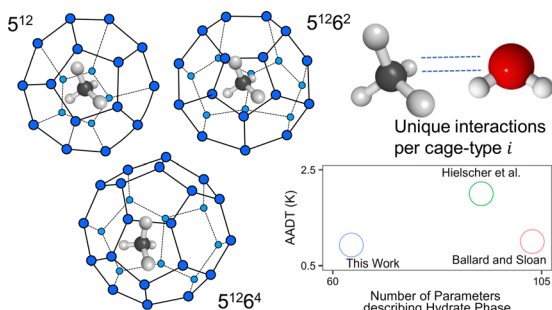
A tetrahydroacridine derivative and its conjugate with gold nanoparticles: promising agents for the treatment of Alzheimer's disease

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



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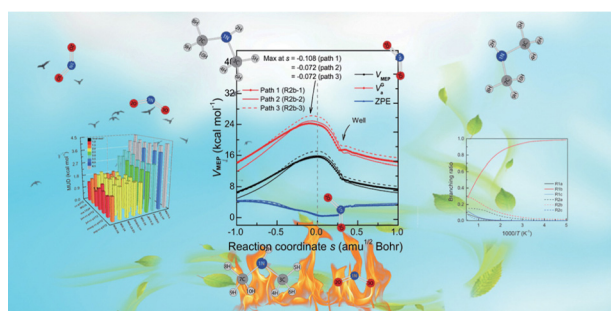
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A cage-specific hydrate equilibrium model for robust predictions of industrially-relevant mixtures

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

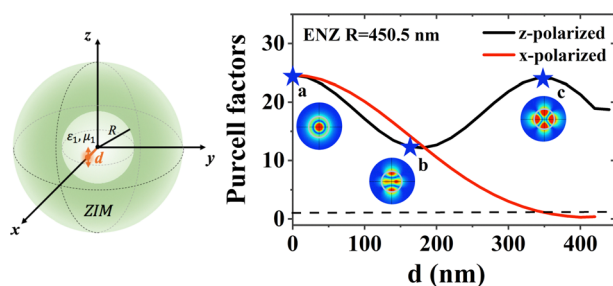
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Advanced kinetic calculations with multi-path variational transition state theory for reactions between dimethylamine and nitrogen dioxide in atmospheric and combustion temperature ranges

Yanlei Shang

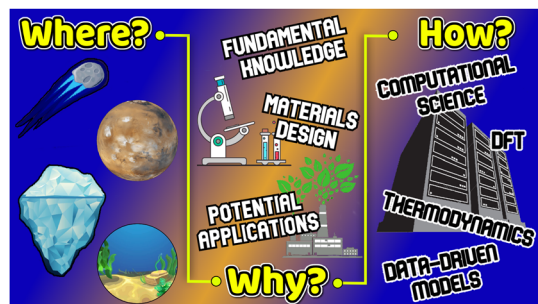
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Inhibition and enhancement of the spontaneous emission in spherical cavities surrounded by zero-index-materials

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-Rodríguez and Rita Prosmiti*

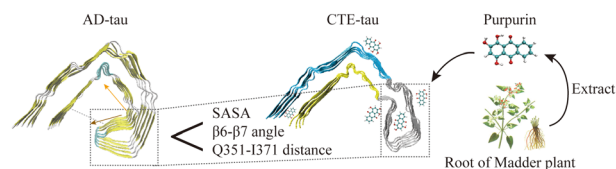


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Destabilization mechanism of R3–R4 tau protofilament by purpurin: a molecular dynamics study

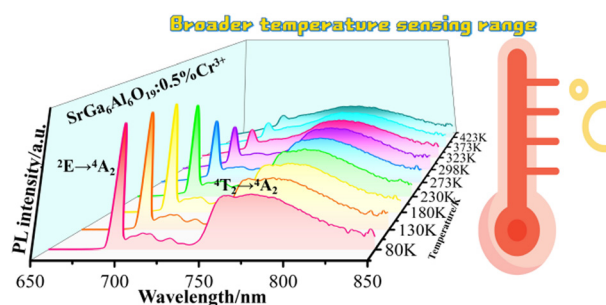
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Extending the optical temperature sensing range of Cr^{3+} by synchronously tuning ${}^2\text{E}$ and ${}^4\text{T}_2$ emission

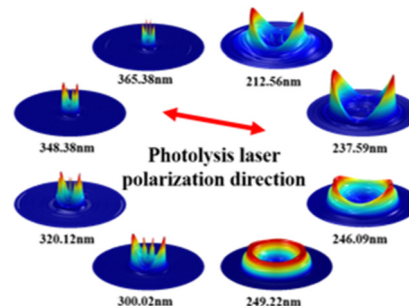
Jiaqi Ou, Shuangqiang Fang,* Qiangqiang Zhu, Yue Zhai, Hong Zhang and Le Wang*



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Slice imaging study of NO_2 photodissociation via the 1^2B_2 and 2^2B_2 states: the $\text{NO}(\text{X}^2\Pi) + \text{O}(\text{P}_j)$ product channel

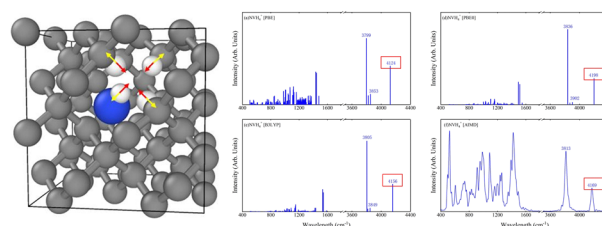
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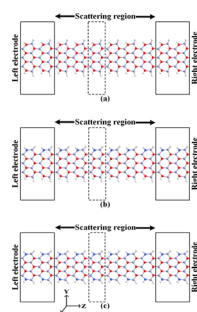
The search for a band of a defect predicted above 4000 cm^{-1} in diamond through infrared vibrational spectra: a quantum mechanical investigation

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



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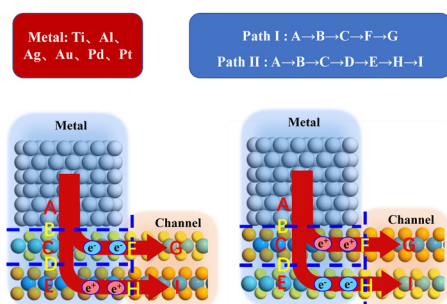
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Nitrogen-doped zinc oxide nanoribbons for potential resonant tunneling diode applications

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

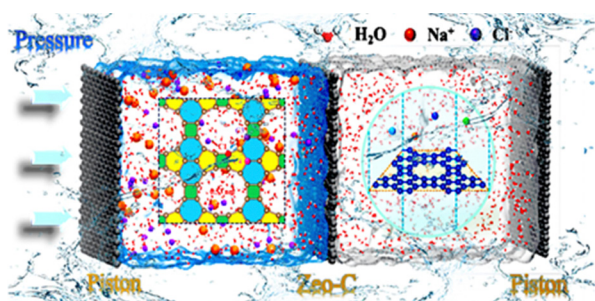
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Dual transmission channels at metal–MoS₂/WSe₂ hetero-bilayer interfaces

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

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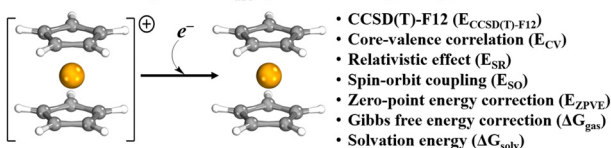


Computational simulation-driven discovery of novel zeolite-like carbon materials as seawater desalination membranes

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

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

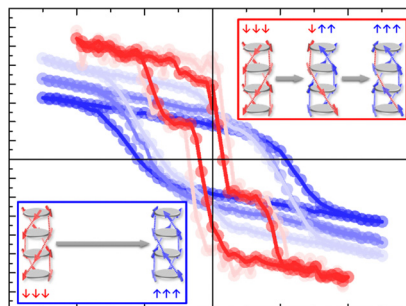


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Ferro- and ferrielectricity and negative piezoelectricity in thioamide-based supramolecular organic discotics

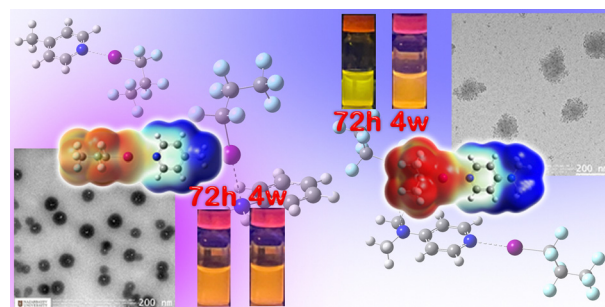
Indre Urbanaviciute, Miguel Garcia-Iglesias, Andrey Gorbunov, E. W. Meijer and Martijn Kemerink*



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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

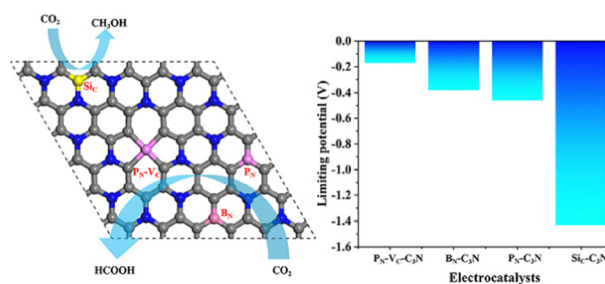
Haiyan Fan, Lazzat Nurtay, Nurgul Daniyeva and Enrico Benassi*



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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

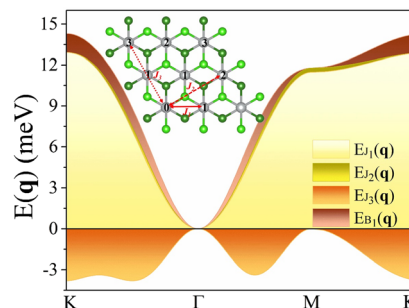
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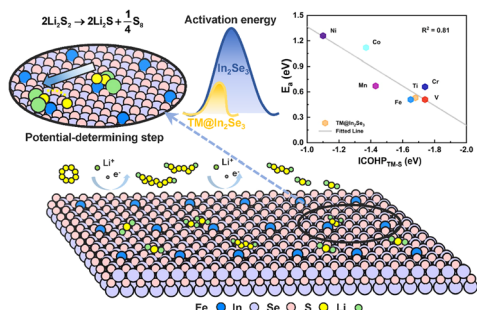
Same effect of biquadratic exchange interaction and Heisenberg linear interaction in a spin spiral

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



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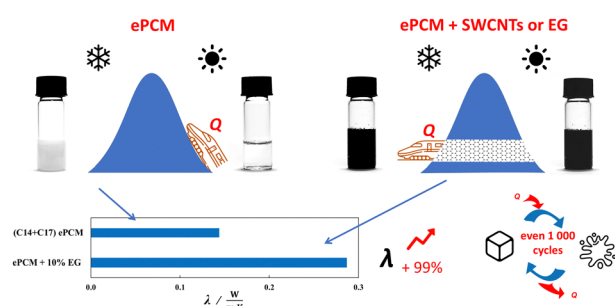
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Identification of linear scaling relationships in polysulfide conversion on α - In_2Se_3 -supported single-atom catalysts

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

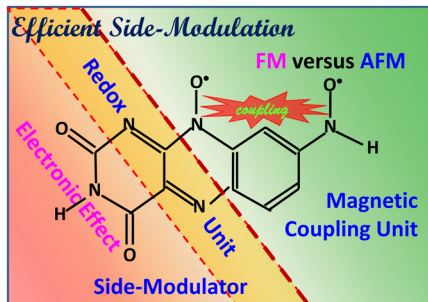
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Alkane-based eutectic phase change materials doped with carbon nanomaterials

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

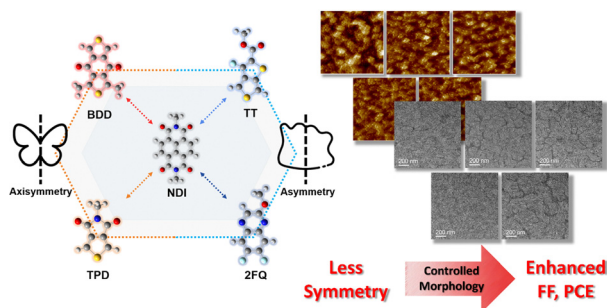
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Magnetic coupling modulation in *meta*-nitroxide-functionalized isoalloxazine magnets with redox-active units as efficient side-modulators

Rabia Malik and Yuxiang Bu*

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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*

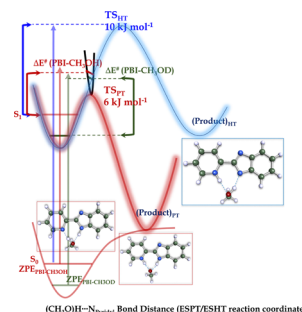


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A combined spectroscopic and computational investigation on the solvent-to-chromophore excited-state proton transfer in the 2,2'-pyridylbenzimidazole–methanol complex

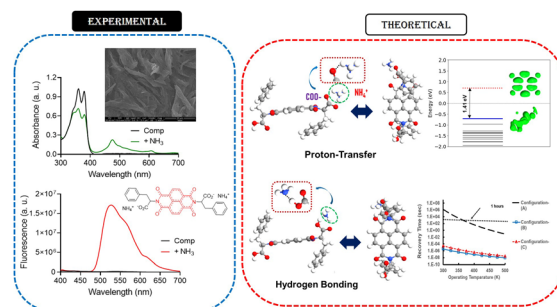
Ramesh Jarupula, Saurabh Khodia, Muhammed Shabeeb and Surajit Maity*



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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

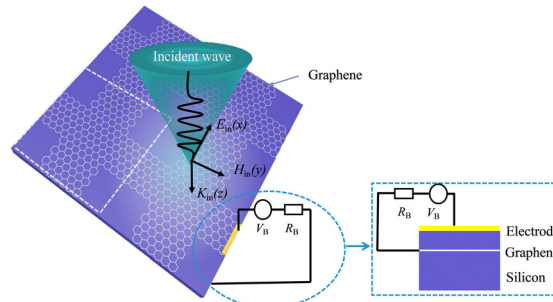
Aditya Tiwari, Rikitha S. Fernandes, Nilanjan Dey* and Sayan Kanungo*



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*

