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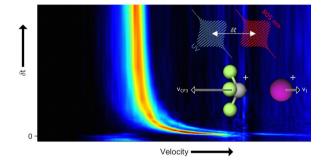
See Michael N. R. Ashfold et al., pp. 16672-16698. Image reproduced by permission of Stuart Crane from Phys. Chem. Chem. Phys., 2023, **25**, 16672.

PERSPECTIVE

16672

Molecular photodissociation dynamics revealed by Coulomb explosion imaging

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

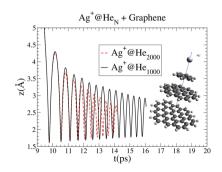


COMMUNICATIONS

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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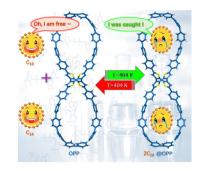
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COMMUNICATIONS

16707

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

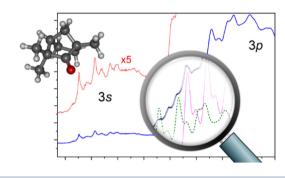
Zeyu Liu,* Xia Wang, Tian Lu,* Jiaojiao Wang, Xiufen Yan, Yang Wu and Jingbo Xu



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

Ivan Powis* and Dhirendra P. Singh

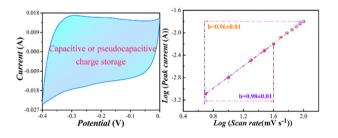


RESEARCH PAPERS

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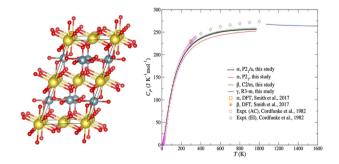
What about electrochemical behaviors for aurivillius-phase bismuth tungstate? Capacitive or pseudocapacitive

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

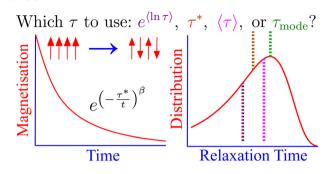


Polymorphism and phase transitions in Na₂U₂O₇ from density functional perturbation theory

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



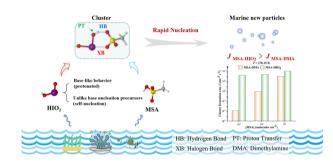
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Characterisation of magnetic relaxation on extremely long timescales

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

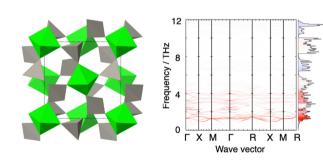
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Methanesulfonic acid and iodous acid nucleation: a novel mechanism for marine aerosols

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

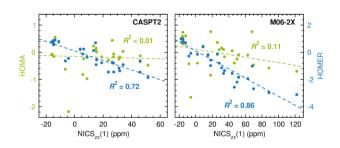
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Phonon mechanism for the negative thermal expansion of zirconium tungstate, ZrW2O8

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

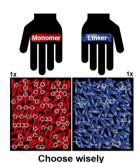
Ismael A. Elayan and Alex Brown*

$$\begin{array}{c|c} \hline \\ \omega_1 \\ \hline \\ \omega_1 \\ \hline \\ \omega_1 \\ \hline \\ D-2PA \\ |0> \end{array} \begin{array}{c|c} R_3 \\ \hline \\ R_4 \\ \hline \\ \hline \\ ND-2PA \\ |0> \end{array} \begin{array}{c|c} |1> \\ \hline \\ \omega_2 \\ \hline \\ \hline \\ ND-2PA \\ |0> \end{array}$$

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Rationalizing the formation of porosity in mechanochemically-synthesized polymers

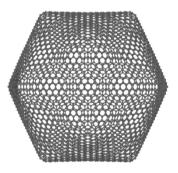
Annika Krusenbaum, Steffi Krause Hinojosa, Sven Fabig, Valentin Becker, Sven Grätz and Lars Borchardt*



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The largest fullerene

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

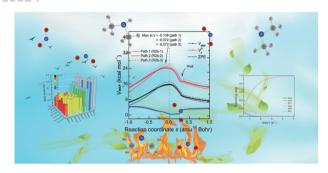
Ilona Mojzych, Anna Zawadzka, Katarzyna Kaczyńska, Piotr Wojciechowski, Dominika Zając, Maciej Chotkowski, Katarzyna Wiktorska, Jan K. Maurin and Maciej Mazur*

16807 Unique interactions per cage-type i Hielscher et al Ballard and Sloar Number of Parameters describing Hydrate Phase

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*

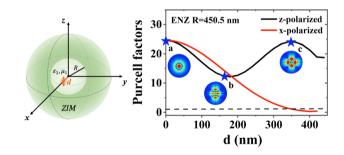
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Advanced kinetic calculations with multi-path variational transition state theory for reactions between dimethylamine and nitrogen dioxide in atmospheric and combustion temperature ranges

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, Xinchen Zhang, Yali Jia, Qihuang Gong and Ying Gu*

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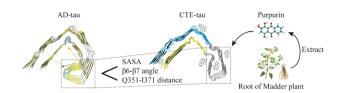
Computational investigations of stable multiplecage-occupancy He clathrate-like hydrostructures

Raquel Yanes-Rodríguez and Rita Prosmiti*

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

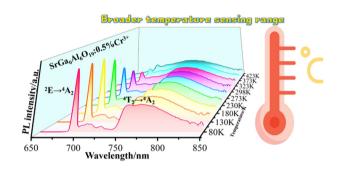
Jiagian Wan, Yu Zou, Ruiging Sun, Zhengdong Xu, Jiaxing Tang, Yehong Gong, Guanghong Wei* and Qingwen Zhang*



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

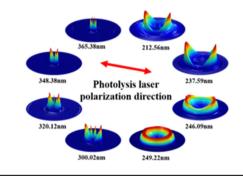
Jiaqi Ou, Shuangqiang Fang,* Qiangqiang Zhu, Yue Zhai, Hong Zhang and Le Wang*



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Slice imaging study of NO₂ photodissociation via the 1^2B_2 and 2^2B_2 states: the NO(X² Π) + O(3P_J) product channel

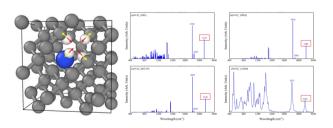
Zhaoxue Zhang, Shuaikang Yang, Zhenxing Li,* Yao Chang, Zijie Luo, Yarui Zhao, Shengrui Yu,* Kaijun Yuan* and Xueming Yang



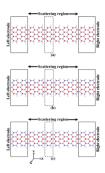
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The search for a band of a defect predicted above 4000 cm⁻¹ in diamond through infrared vibrational spectra: a quantum mechanical investigation

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



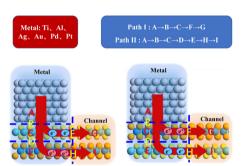
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Nitrogen-doped zinc oxide nanoribbons for potential resonant tunneling diode applications

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

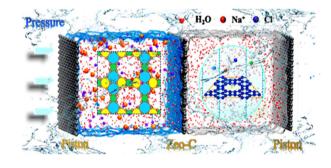
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Dual transmission channels at metal-MoS₂/WSe₂ hetero-bilayer interfaces

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

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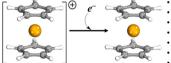


Computational simulation-driven discovery of novel zeolite-like carbon materials as seawater desalination membranes

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

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Absolute reduction potential ($\mathring{E_{abs}}$) predictions for Cp_2M^+/Cp_2M (M=Fe, Co and Ni)



- CCSD(T)-F12 (E_{CCSD(T)-F12}) Core-valence correlation (E_{CV})
- Relativistic effect (E_{SR})
- Spin-orbit coupling (E_{SO})
- Zero-point energy correction (E_{ZPVE})
- Gibbs free energy correction (ΔG_{gas})
- Solvation energy (ΔG_{solv})

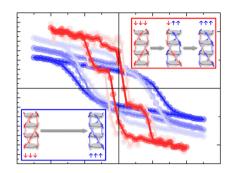
Ferrocene/ferrocenium, cobaltocene/ cobaltocenium and nickelocene/nickelocenium: from gas phase ionization energy to one-electron reduction potential in solvated medium

Hongyan Zhao, Yi Pan and Kai-Chung Lau*

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

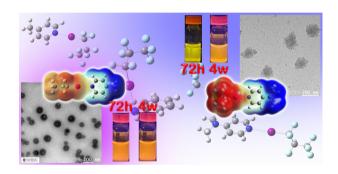
Indre Urbanaviciute, Miguel Garcia-Iglesias, Andrey Gorbunov, E. W. Meijer and Martijn Kemerink*



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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

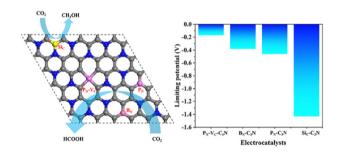
Haiyan Fan, Lazzat Nurtay, Nurgul Daniyeva and Enrico Benassi*



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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

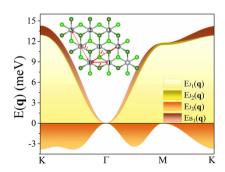
Dandan Wang, Xueting Liu, Huiru Yang, Ziang Zhao, Yucheng Liu, Xin Qu, Lihua Yang, Ming Feng* and Zaicheng Sun*



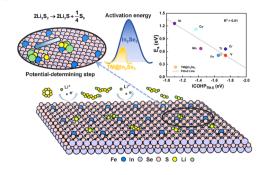
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Same effect of biquadratic exchange interaction and Heisenberg linear interaction in a spin spiral

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



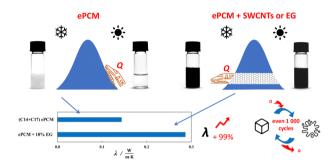
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Identification of linear scaling relationships in polysulfide conversion on α-In₂Se₃-supported single-atom catalysts

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

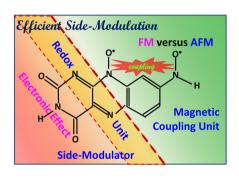
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Alkane-based eutectic phase change materials doped with carbon nanomaterials

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

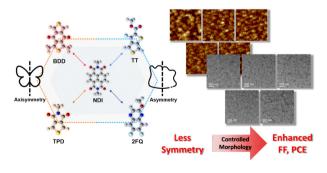
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Magnetic coupling modulation in meta-nitroxidefunctionalized isoalloxazine magnets with redox-active units as efficient side-modulators

Rabia Malik and Yuxiang Bu*

17001



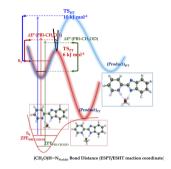
Naphthalene diimide-based random terpolymers with axisymmetric and asymmetric electron acceptors for controllable morphology and enhanced fill factors in all-polymer solar cells

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

17010

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

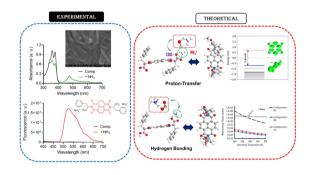
Ramesh Jarupula, Saurabh Khodia, Muhammed Shabeeb and Surajit Maity*



17021

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

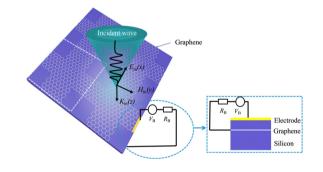
Aditya Tiwari, Rikitha S. Fernandes, Nilanjan Dey* and Sayan Kanungo*



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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*

