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ISSN 1463–9076 CODEN PPCPFQ 25(17) 11861–12534 (2023)



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EDITORIAL

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Festschrift for Wolfgang E. Ernst – electronic and nuclear dynamics and their interplay in molecules, clusters and on surfaces

Andreas W. Hauser, Martina Havenith, Markus Koch and Martin Sterrer

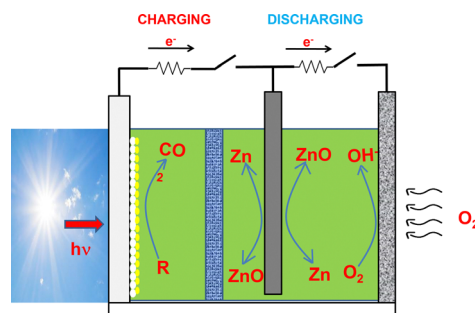


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A brief review on solar charging of Zn–air batteries

Panagiotis Lianos



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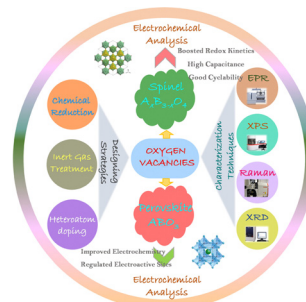
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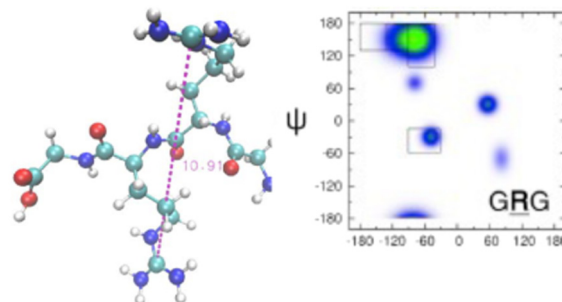


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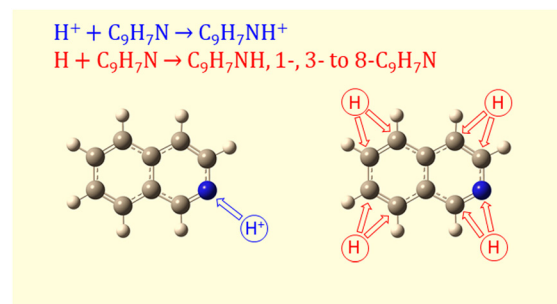


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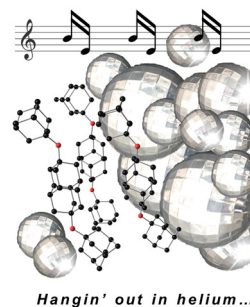


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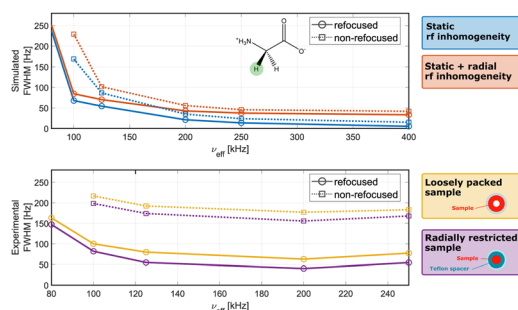
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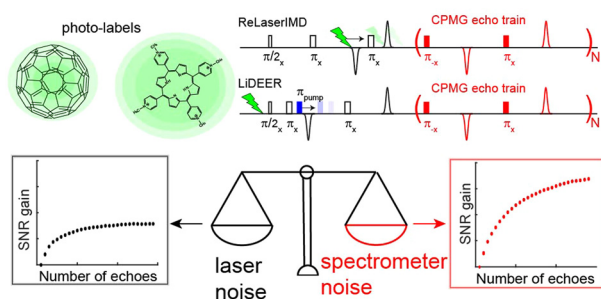
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Residual proton line width under refocused frequency-switched Lee-Goldburg decoupling in MAS NMR

Kathrin Aebischer and Matthias Ernst*

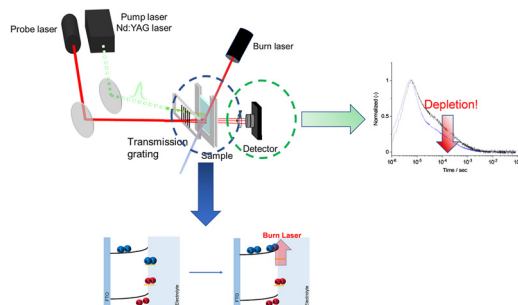
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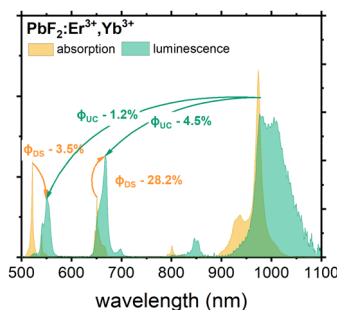
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Development of charge carrier-selective heterodyne transient grating spectroscopic technique and its application in the distinction of surface trap states in hematite

Young Hyun Kim, Yu Gyeong Bae and Woon Yong Sohn*

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Absolute quantum yield for understanding upconversion and downshift luminescence in PbF₂:Er³⁺,Yb³⁺ crystals

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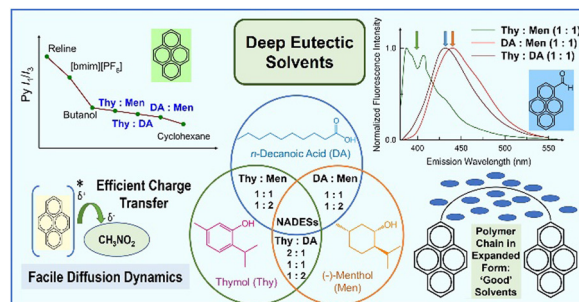


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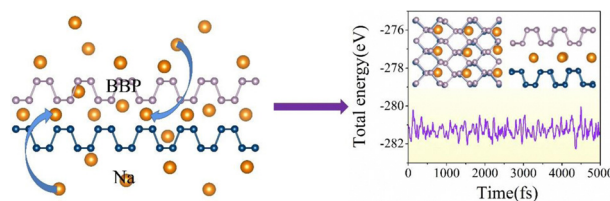
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A first-principles study of bilayered black phosphorene as a potential anode material for sodium-ion batteries

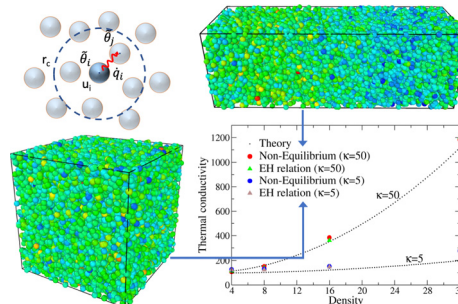
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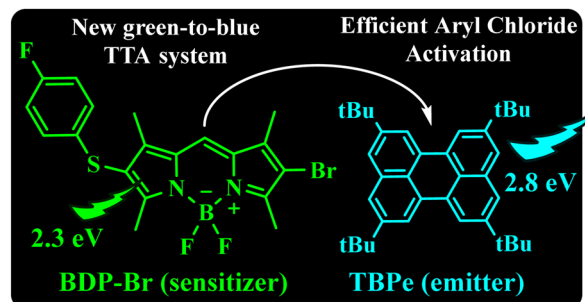
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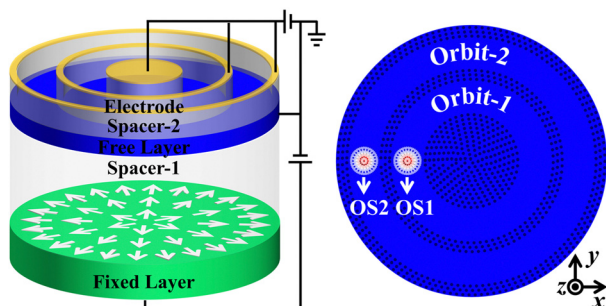
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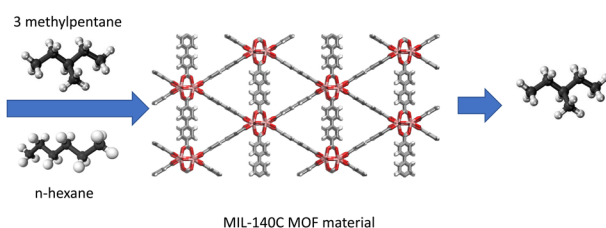
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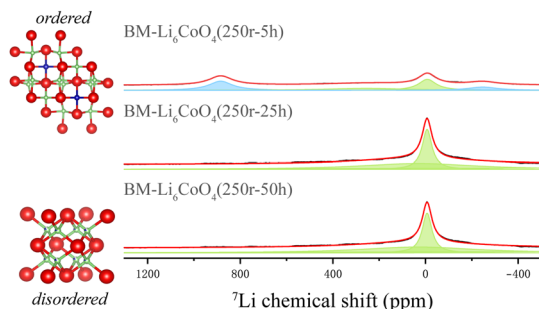
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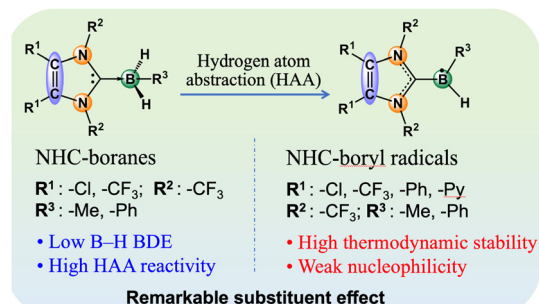
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**Formation and reactivity of NHC-boryl radicals: insight into substituent effect from theoretical calculations**

Lin Zhang and Zexing Cao*

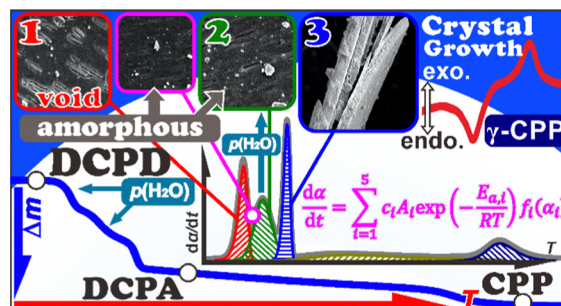


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Physico-geometrical kinetic insight into multistep thermal dehydration of calcium hydrogen phosphate dihydrate

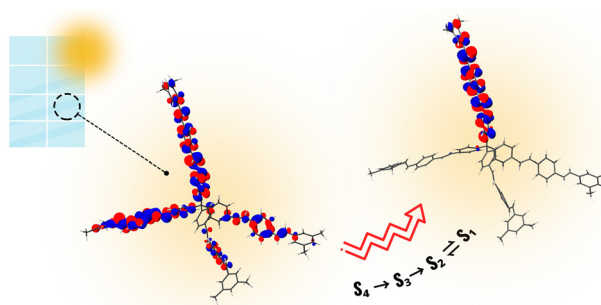
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Impact of the core on the inter-branch exciton exchange in dendrimers

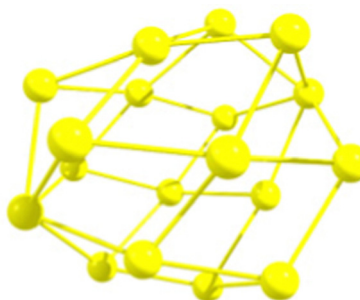
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Engineering magic number Au₁₉ and Au₂₀ cage structures using electron withdrawing atoms

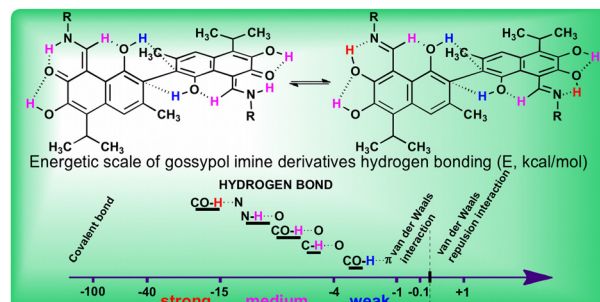
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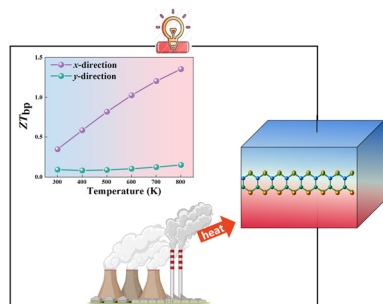
Intramolecular hydrogen bonds of gossypol imine derivatives

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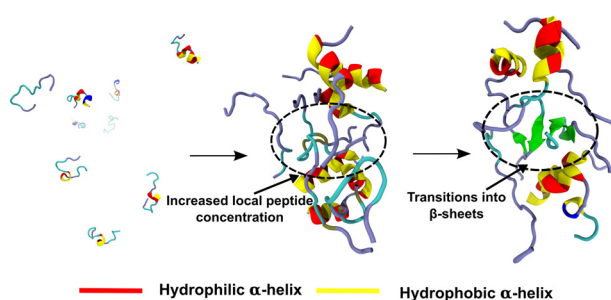
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Electron–phonon coupling, bipolar effects, and thermoelectric performance of the CuSbS₂ monolayer

Ao-Dong Chen, Chuan-Lu Yang,* Mei-Shan Wang and Xiao-Guang Ma

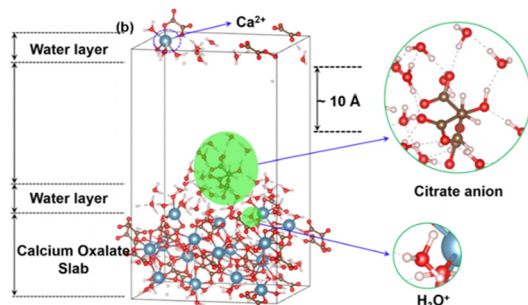
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Helical intermediate formation and its role in amyloids of an amphibian antimicrobial peptide

Anup Kumar Prasad, Lisandra L. Martin and Ajay S. Panwar*

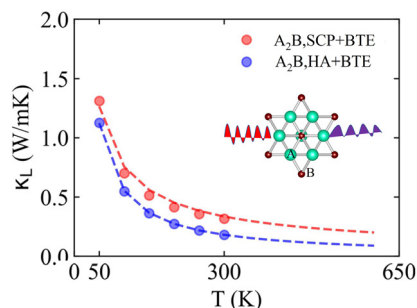
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A molecular understanding of citrate adsorption on calcium oxalate polyhydrates

Yangyang Su, Jelle Vekeman, Flavio Siro Brigiano, Etienne Paul Hessou, Yuheng Zhao, Diane Sorgeloos, Marc Raes, Tom Hauffman, Kehzi Li and Frederik Tielens*

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Ultralow lattice thermal conductivity of binary compounds A₂B (A = Cs, Rb & B = Se, Te) with higher-order anharmonicity correction

Shuming Zeng,* Lei Fang, Yusong Tu, M. Zulfiqar* and Geng Li*

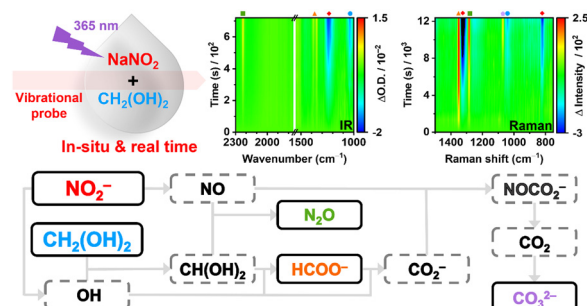


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In situ and real-time vibrational spectroscopic characterizations of the photodegradation of nitrite in the presence of methanediol

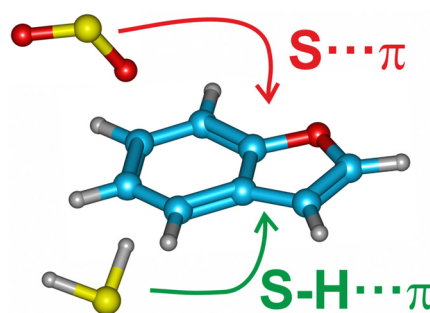
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Sulfur–arene interactions: the $S \cdots \pi$ and $S-H \cdots \pi$ interactions in the dimers of benzofuran $\cdots$ sulfur dioxide and benzofuran $\cdots$ hydrogen sulfide

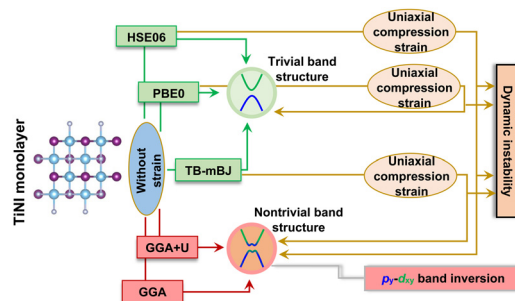
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New insights into band inversion and topological phase of TiNi monolayer

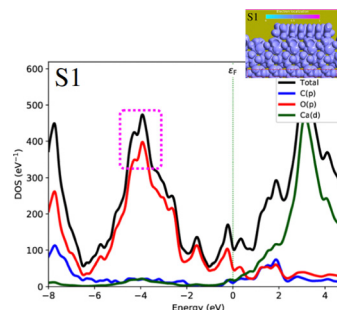
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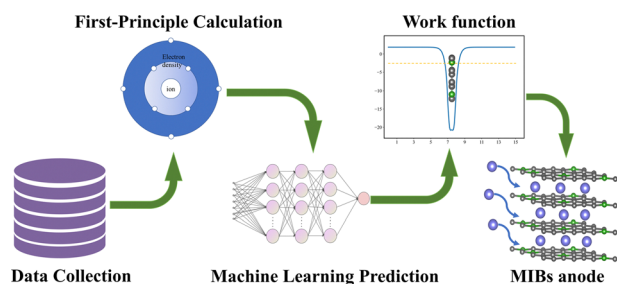
Unravelling the impact of oily alkane molecules on the optical properties of the calcite(10.4) surface

Junais Habeeb Makkath



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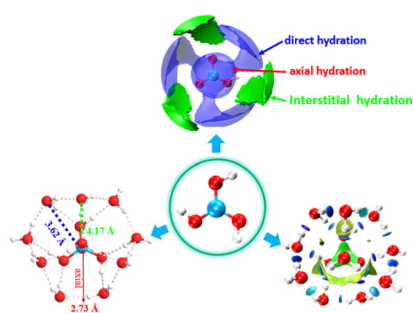
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Machine-learning-assisted discovery of boron-doped graphene with high work function as an anode material for Li/Na/K-ion batteries

Yi Luo, Haiyuan Chen,* Jianwei Wang and Xiaobin Niu

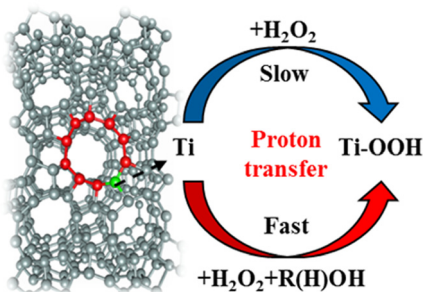
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Structural analysis of potassium borate solutions

Fayan Zhu, Daniel T. Bowron, Sabrina Gärtner, Chunhui Fang, Yongquan Zhou, Hongyan Liu and Alex C. Hannon*

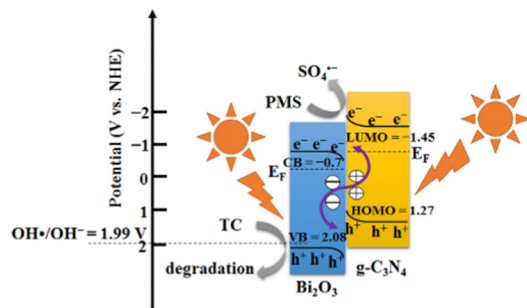
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Evidence of solvent-mediated proton transfer during H₂O₂ activation in titanosilicate-catalyzed oxidation systems

Yunkai Yu, Jianhao Wang, Nan Fang, Zhen Chen, Dongxu Liu, Yueming Liu* and Mingyuan He

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A 1D/2D Bi₂O₃/g-C₃N₄ step-scheme photocatalyst to activate peroxymonosulfate for the removal of tetracycline hydrochloride: insight into the mechanism, reactive sites, degradation pathway and ecotoxicity

Mingyang Long, Di Li,* Qianqian Zhao, Hongmiao Li, Qi Wen, Li Wang, Lei Wu, Fang Song and Jun Zhou

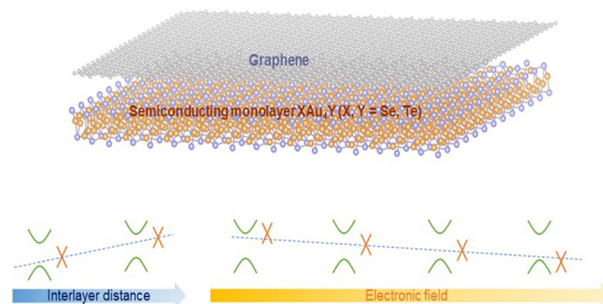


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Tunable Schottky contacts in graphene/XAu₄Y (X, Y = Se, Te) heterostructures

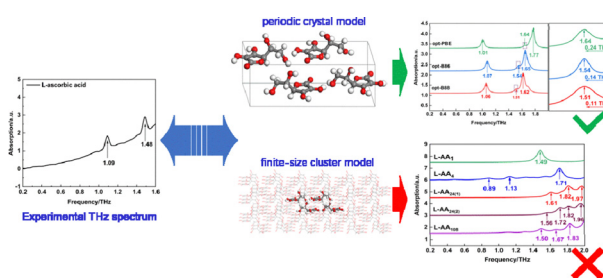
Yufei Xue, Lei Gao,* Weina Ren, Xuxia Shai, Tingting Wei, Chunhua Zeng* and Hua Wang*



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First principles terahertz spectroscopy of molecular crystals: the crucial role of periodic boundary conditions benchmarked with experimental L-ascorbic acid spectra

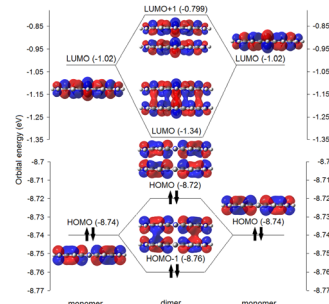
Ying Wang, Huifang Ma, Yanzhao Yang, Jiantao Qi, Guiming Zhang, Hao Ren* and Wenye Guo*



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Theoretical study of the excitation of proflavine H-dimers in an aqueous solution: the effect of functionals and dispersion corrections

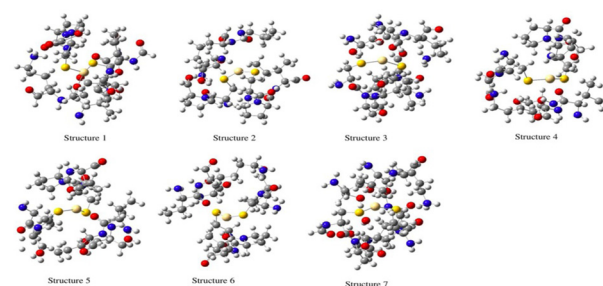
Evgeniy S. Savenko and Victor V. Kostjukov*



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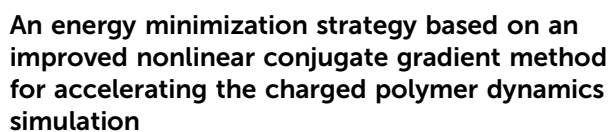
Calculation of electric field gradients in Cd(II) model complexes of the CueR protein metal site

Catriona A. O'Shea, Rasmus Fromsejer, Stephan P. A. Sauer, Kurt V. Mikkelsen* and Lars Hemmingsen*





12290



12308



12322

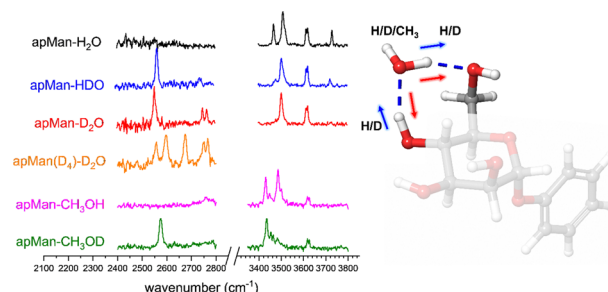
11874 | *Phys. Chem. Chem. Phys.*, 2023, **25**, 11863–11879

RESEARCH PAPERS

12331

Isotopic dependence of intramolecular and intermolecular vibrational couplings in cooperative hydrogen bond networks: singly hydrated phenyl- α -D-mannopyranoside as a case study

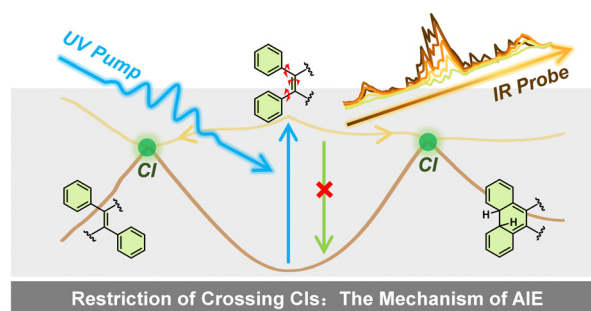
Ander Camiruaga, Gildas Goldsztejn and Pierre Çarçabal*



12342

Restriction of crossing conical intersections: the intrinsic mechanism of aggregation-induced emission

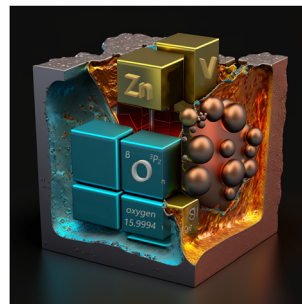
Jie Peng, Xin He, Yao Li, Jianxin Guan, Baihua Wu, Xinmao Li, Zhihao Yu, Jian Liu* and Junrong Zheng*



12352

First principles calculation of the $\text{ZnV}_2\text{O}_6(001)$ surface terminations: the thermodynamic stability and electronic structure study

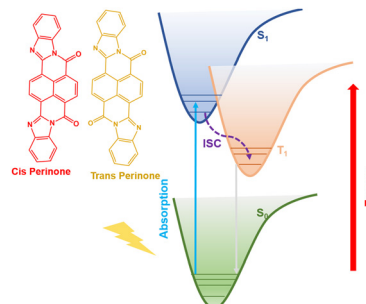
Anqi Yang, Jiaolian Luo,* Zhenyu Xie, Qian Chen* and Quan Xie



12363

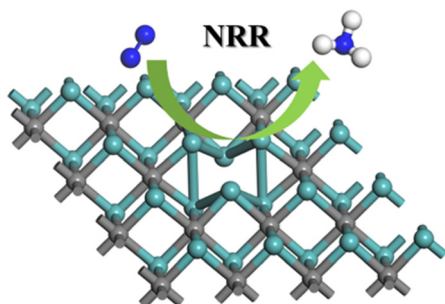
Probing the excited state dynamics in perinone molecules for photovoltaic applications using transient absorption spectroscopy

Suman Dhami, Yogesh Kumar, Chaitrali Sengupta and Ravindra Pandey*



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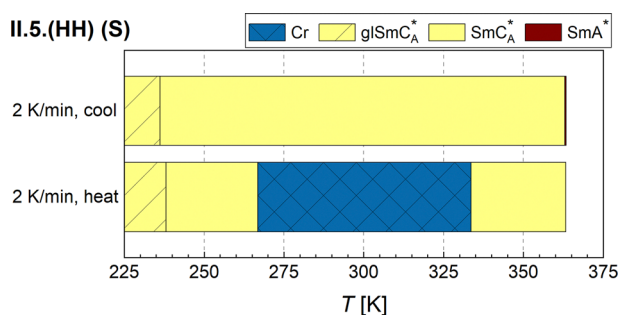
12371



Defective Mo₂C as a promising electrocatalyst for the nitrogen reduction reaction

Xuanyue Zhang, Tingting Zhao, Likai Yan* and Zhongmin Su

12379

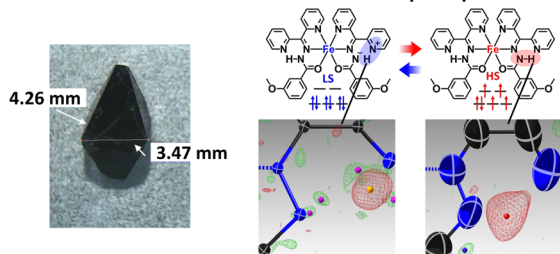


Vitrification of the smectic C_A* phase and kinetics of cold crystallization investigated for a fluorinated compound with a chiral centre based on (S)-(+)-3-octanol

Aleksandra Deptuch,* Artur Lelito, Ewa Juszyńska-Gałązka, Małgorzata Jasiurkowska-Delaporte and Magdalena Urbańska

12394

Proton Tautomerism Based on Proton Transfer Coupled Spin Transition

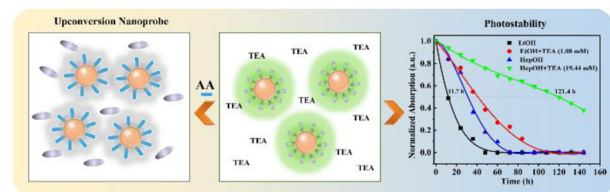


Observation of proton tautomerism by single-crystal neutron diffraction

Observation of proton-transfer-coupled spin transition by single-crystal neutron-diffraction measurement

Takumi Nakanishi, Yuta Hori, Yasuteru Shigeta, Hiroyasu Sato, Shu-Qi Wu, Ryoji Kiyonagi, Koji Munakata, Takashi Ohhara and Osamu Sato*

12401



The effect of triethylamine on dye-sensitized upconversion luminescence and its application in nanoprobe and photostability

Xiao-Bo Zhang, Zuo-Qin Liang,* Xu Yan, Mao-Mao Li, Chang-Qing Ye, Xiao-Mei Wang and Xu-Tang Tao



Tetrel bonds involving a CF₃ group participate in protein–drug recognition: a combined crystallographic and computational study

Protein-drug complex

QM model

PDBID 3POZ

03P
1023

CYS775

TtB

Charge-controlled switchable CO₂ capture and gas separation using BC₃ nanosheets

Theoretical study on the solvation mechanism of camptothecin in ionic liquids

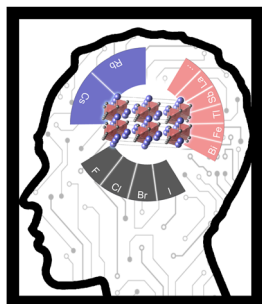
[illegible]

Universal correlation of the superconducting transition temperature with the linear-in-T coefficient, electron packing parameter, and the numbers of valence and conduction electrons

(b) Data fitted with Eq. 6

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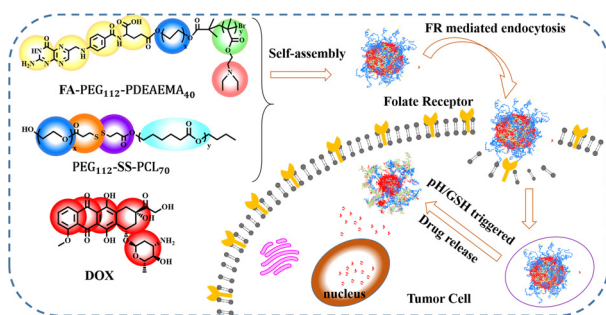
12450



Substitution engineering of lead-free halide perovskites for photocatalytic applications assisted by machine learning

Tao Wang, Shuxin Fan, Hao Jin,* Yunjin Yu and Yadong Wei*

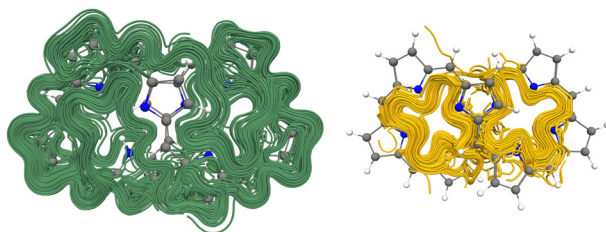
12458



Folate modified dual pH/reduction-responsive mixed micelles assembled using FA-PEG-PDEAEMA and PEG-SS-PCL for doxorubicin delivery

Chufen Yang, Delin Wang, Wenyao Liu, Zexiong Yang, Teng He, Fang Chen and Wenjing Lin*

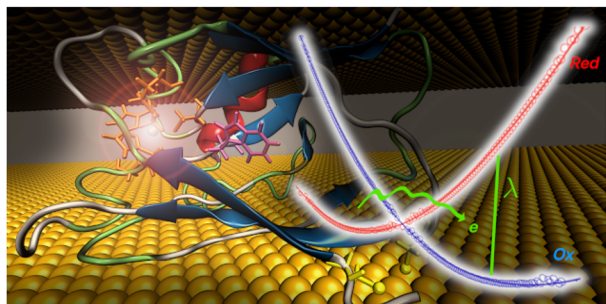
12469



Current-density pathways in figure-eight-shaped octaphyrins

Qian Wang, Jaakko Pykkö, Maria Dimitrova, Stefan Taubert and Dage Sundholm*

12479



Applicability of perturbed matrix method for charge transfer studies at bio/metallic interfaces: a case of azurin

Outi Vilhelmiina Kontkanen, Denys Biriukov and Zdenek Futera*

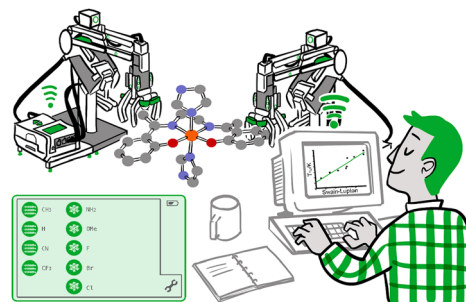


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12490

Fine-tuning of the spin-crossover properties of Fe(III) complexes *via* ligand design

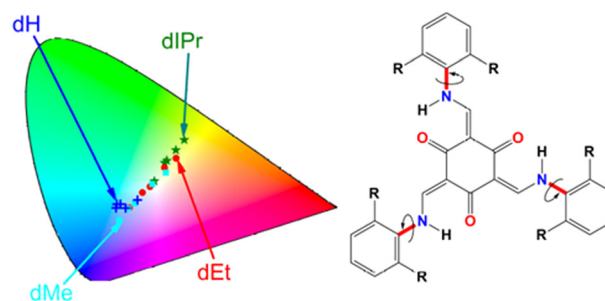
Daniel Vidal, Jordi Cirera* and Jordi Ribas-Arino*



12500

Magnifying the ESIPT process in tris(salicylideneanilines) *via* the steric effect – a pathway to the molecules with panchromatic fluorescence

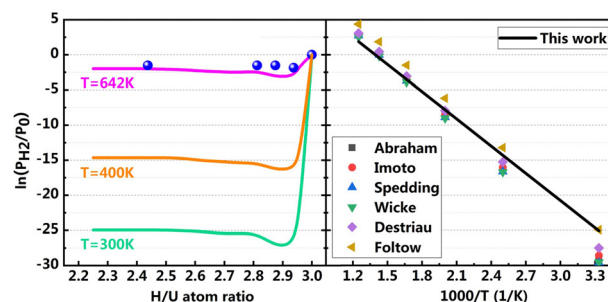
Pawel Gawrys, Olaf Morawski,* Marzena Banasiewicz and Cristina A. Barboza*



12515

Initial decomposition mechanisms and the inverse effects of temperature and P_{H_2} on the thermodynamic stability of UH_3

Le Zhang, Yanhong Zhao, Hongzhou Song, Xingyu Gao, Qili Zhang, Yu Liu, Bo Sun,* Mingfeng Tian, Haifeng Song and Haifeng Liu*



12522

The selective heating effect of microwave irradiation on a binary mixture of water and polyethylene oxide: a molecular dynamics simulation approach

Junhe Chen, Matthew J. Warner, Benjamin Sikora, Daniel Kiddle, Danielle Coverdell, Omar Allam, Paul A. Kohl and Seung Soon Jang*

