

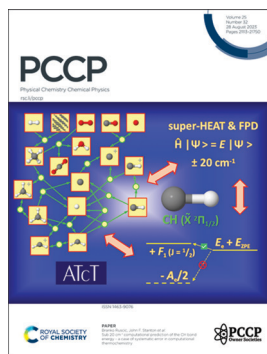
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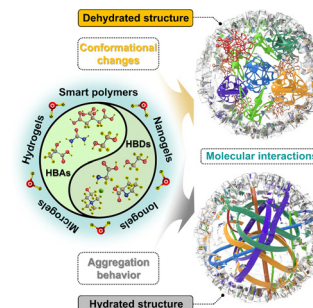
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PERSPECTIVE

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Deep eutectic solvents induced changes in the phase transition behavior of smart polymers: a sustainable future approach

Reddicherla Umapathi, Seyed Majid Ghoreishian, Krishan Kumar, Diksha Dhiman, Gokana Mohana Rani, Yun Suk Huh* and Pannuru Venkatesu*

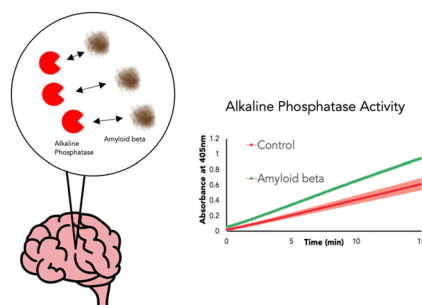


COMMUNICATION

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Interactions with amyloid beta peptide and acetylcholinesterase increase alkaline phosphatase activity

Ashlesha Bhide and Ayusman Sen*



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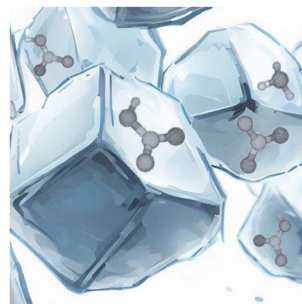


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Does HNO_3 dissociate on gas-phase ice nanoparticles?

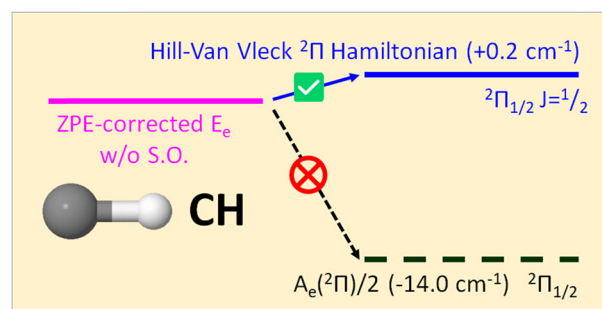
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Sub 20 cm^{-1} computational prediction of the CH bond energy – a case of systematic error in computational thermochemistry

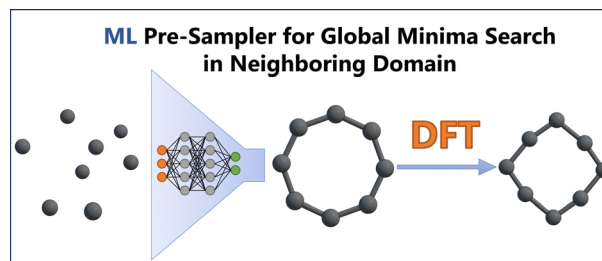
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Neural network atomistic potentials for global energy minima search in carbon clusters

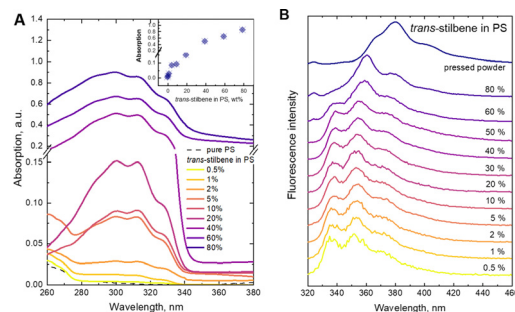
Nikolay V. Tkachenko,* Anastasiia A. Tkachenko,*
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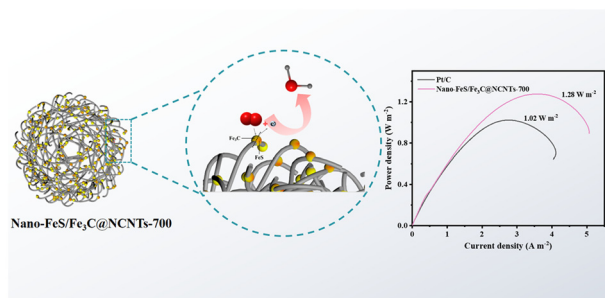
Two phases of *trans*-stilbene in a polystyrene matrix

Renata Karpicz, Gabriele Kareivaite,
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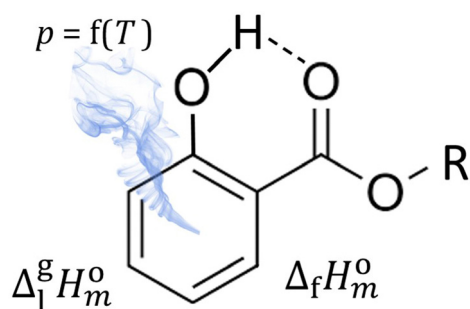
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A facile synthesis of FeS/Fe₃C nanoparticles highly dispersed on *in situ* grown N-doped CNTs as cathode electrocatalysts for microbial fuel cells

Zhuoyue Chen, Yingyu Lin, Yuying Zhou, Yuxian Yang, Yaotang Zhong, Mengqing Xu and Weishan Li*

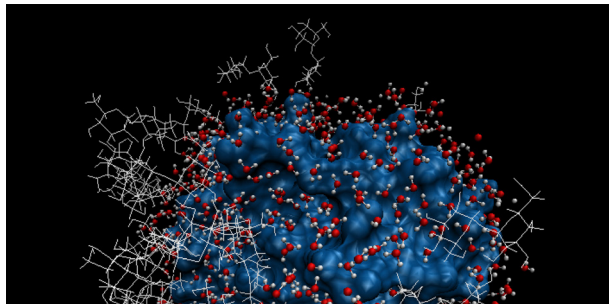
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Experimental and computational thermochemistry: how strong is the intramolecular hydrogen bond in alkyl 2-hydroxybenzoates (salicylates)

Sergey P. Verevkin,* Svetlana V. Portnova, Vladimir N. Emel'yanenko, Ruslan N. Nagrimanov and Mikhail A. Varfolomeev

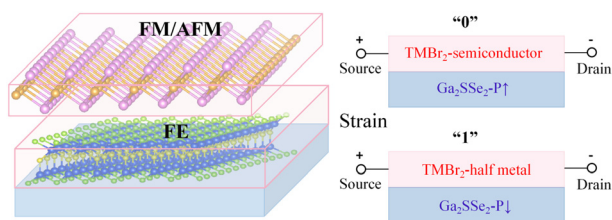
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New insights into the protein stabilizing effects of trehalose by comparing with sucrose

Kajsa Ahlgren, Christoffer Olsson, Inna Ermilova and Jan Swenson*

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The effect of switchable electronic polarization states on the electronic properties of two-dimensional multiferroic TMBR₂/Ga₂SSe₂ (TM = V–Ni) heterostructures

Jinlian Lu, Nini Guo, Yuanyuan Duan, Shu Wang, Yuxuan Mao, Sun Yi, Lijuan Meng, Xiaojing Yao and Xiuyun Zhang*

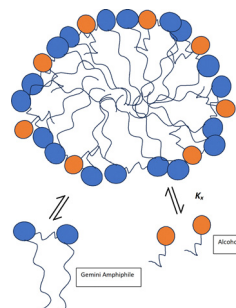


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The partitioning of primary alcohols into the aggregates of gemini amphiphiles determined from diffusion NMR experiments

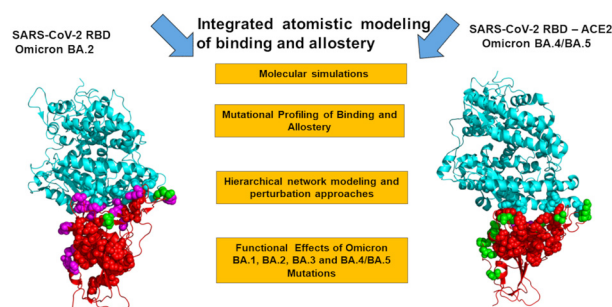
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Probing conformational landscapes of binding and allostery in the SARS-CoV-2 omicron variant complexes using microsecond atomistic simulations and perturbation-based profiling approaches: hidden role of omicron mutations as modulators of allosteric signaling and epistatic relationships

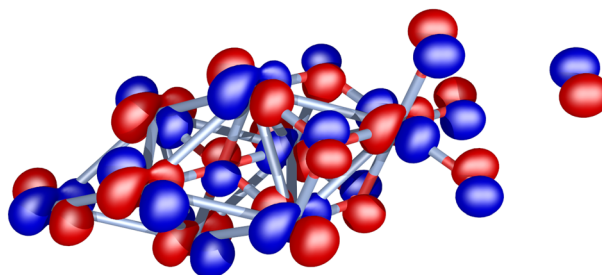
Gennady Verkhivker,* Mohammed Alshahrani, Grace Gupta, Sian Xiao and Peng Tao



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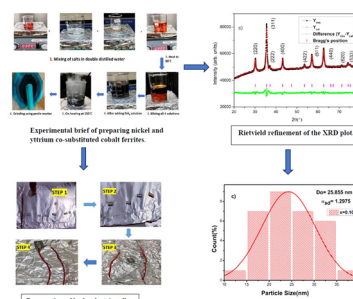
Pavel Pokhilko* and Dominika Zgid



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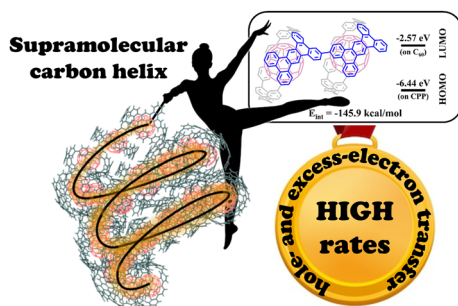
Unveiling the impact of Ni²⁺/Y³⁺ co-substitution on the structural, dielectric, and impedance properties of multiferroic spinel ferrite for hydroelectric cell application

Prachi Jain, S. Shankar* and O. P. Thakur*



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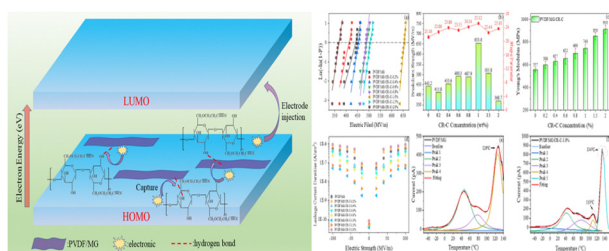
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Photoinduced electron transfer in [10]CPP-C₆₀ oligomers with stable and well-defined supramolecular structures

A. J. Stasyuk

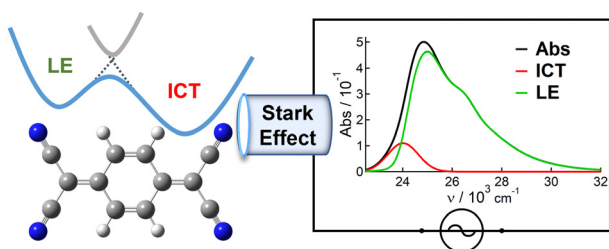
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All-organic PVDF-based composite films with high energy density and efficiency synergistically tailored by MMA-co-GMA copolymer and cyanoethylated cellulose

Junhao Xie, Xuanchen Zhao, Shuo Zheng, Shaoyuan Zhong, Xiaomeng Liu, Mingyao Zhang* and Shulin Sun*

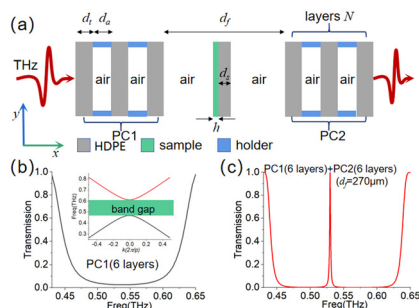
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Charge-transfer state and state mixing in tetracyanoquinodimethane probed using electroabsorption spectroscopy

Ahatashamul Islam, Kensuke Syundo and Toshifumi Iimori*

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Boosting of the terahertz absorption spectrum based on one-dimensional plastic photonic crystals

Xiangjun Li, Ding Ding, Dexian Yan,* Jianjun Liu and Le Zhang

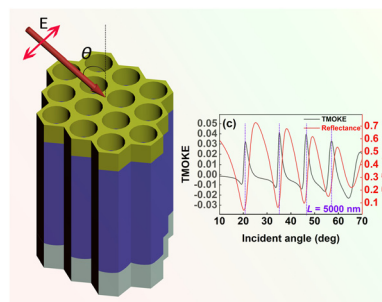


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Transverse magneto-optical behavior of nanoporous ferromagnetic film based on anodic aluminum oxide/aluminum template and its sensing application

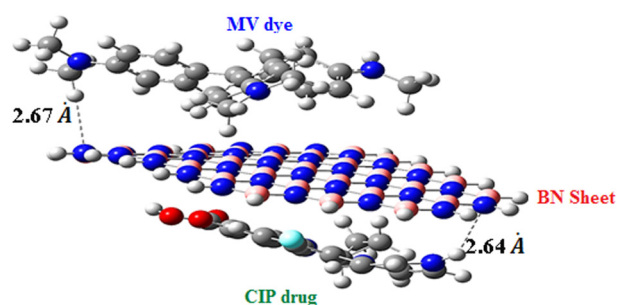
Guoqiang Du, Pingping Zheng, Na Liu, Zhifeng Liu, Lin Zhang and Weiwei Zhang*



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Simultaneous adsorption of ciprofloxacin drug and methyl violet dye on boron nitride nanosheets: experimental and theoretical insights

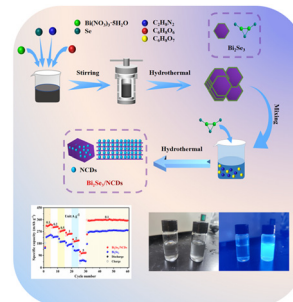
Keivan Javanmard, Saeed Farhadi* and Abedin Zabardasti*



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Facile synthesis of Bi_2Se_3 /nitrogen-doped carbon dot nanoplates for aqueous zinc ion battery cathodes

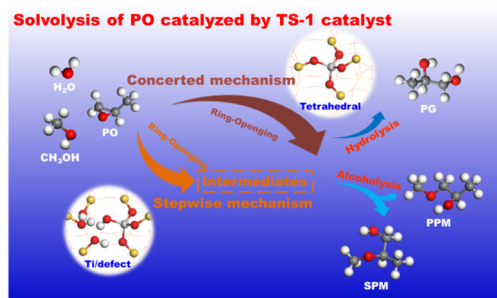
Yuxin Han, Hongfang Jiu,* Lixin Zhang,* Cundong Wang,* Luchao Yue, Congli Wang, Zhixin Guo, Sicong Che, Jinfeng Ma and Hui Li



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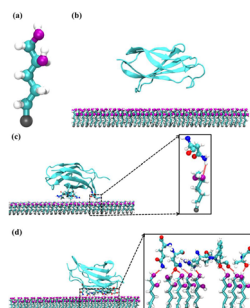
Insights into the mechanism of the solvolysis of propylene oxide over titanium silicalite-1: a theoretical study

Qiaoyun Qin, Hongxia Liu, Yanke Guo, Baohe Wang, Jing Zhu* and Jing Ma*



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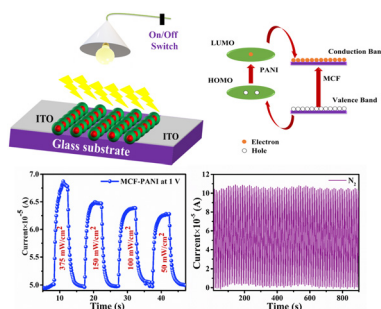
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Unexpectedly resisting protein adsorption on self-assembled monolayers terminated with two hydrophilic hydroxyl groups

Dangxin Mao, Yuan-Yan Wu* and Yusong Tu*

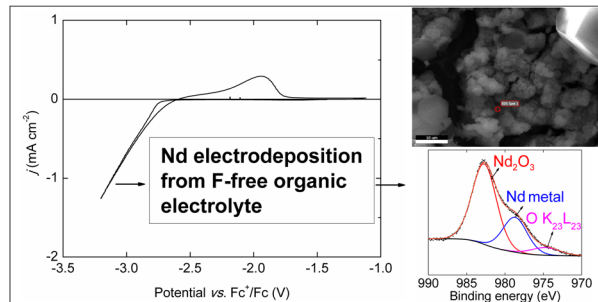
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An investigation into the hybrid architecture of Mn–Co nanoferrites incorporated into a polyaniline matrix for photoresponse studies

Anshika Singh,* Pratima Chauhan, Arpit Verma and B. C. Yadav

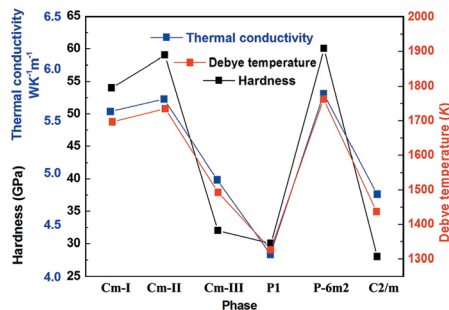
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Fluorine-free organic electrolytes for the stable electrodeposition of neodymium metal

Pieter Geysens, Da Tie, Alexandru Vlad, Jan Fransaer and Koen Binnemans*

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Superhard bulk C₄N₃ compounds with metal-free magnetism assembled from two-dimensional C₄N₃: a first-principles study

Haiping Wu,* Yuelin Li, Yan Qian* and Erjun Kan

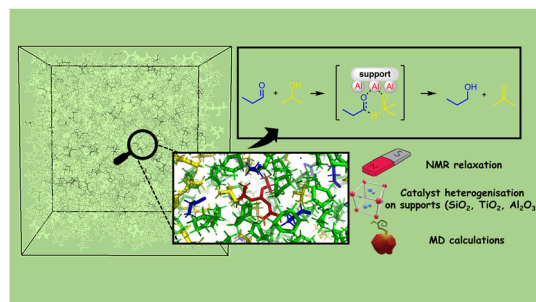


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Heterogenised catalysts for the H-transfer reduction reaction of aldehydes: influence of solvent and solvation effects on reaction performances

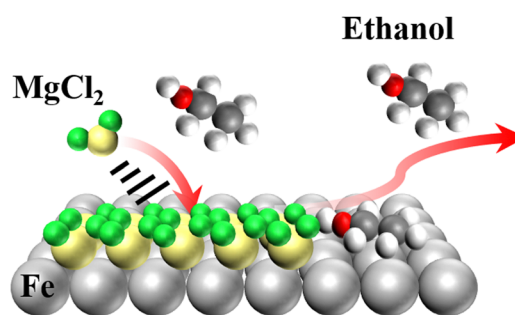
Atika Muhammad, Chengxu Zhu, Xiao Yu, Graziano Di Carmine, Hannah Wood, Paola Carbone, Sam P. de Visser, Christopher Hardacre and Carmine D'Agostino*



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Unexpected higher corrosion in the gas phase region of metals caused by calcium and magnesium ions compared to sodium ions

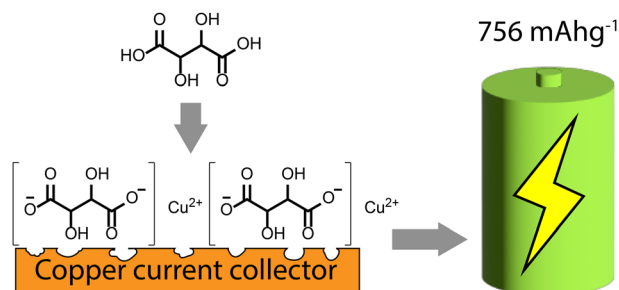
Yi Luo, Zhenglin He, Huayan Yang, Yunzhang Li, Dongting Yue, Zehui Zhang and Guosheng Shi*



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Formulation and mechanism of copper tartrate – a novel anode material for lithium-ion batteries

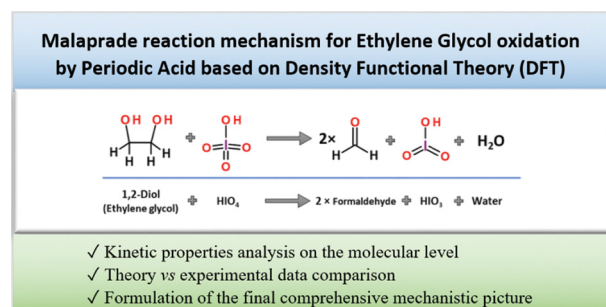
Matthew Teusner, Uttam Mittal, Martina Lessio, Bernt Johannessen, Jitendra Mata and Neeraj Sharma*



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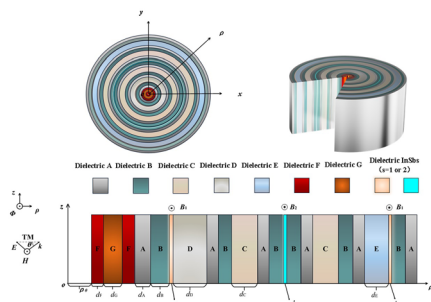
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Agata Kołodziejczyk, Mikołaj Błaziak, Kinga Podgórnaiak, Aneta Jezierska and Kacper Błaziak*



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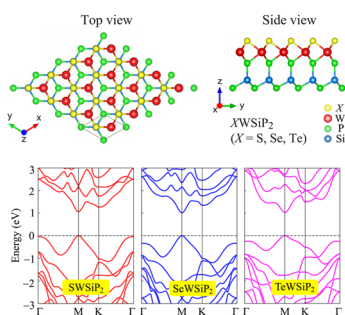
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The multiple physical quantity sensor based on cylindrical photonic crystals with XOR logic gates

Ding-Yuan Zhang, Jun-Yang Sui, You-Ming Liu and Hai-Feng Zhang*

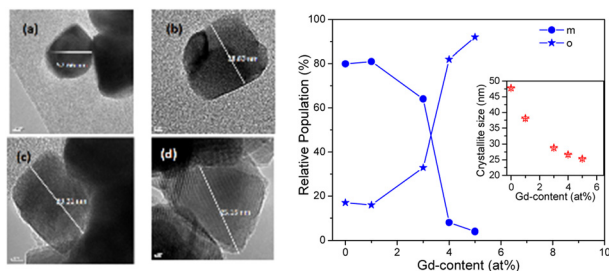
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Moderate direct band-gap energies and high carrier mobilities of Janus $XWSiP_2$ ($X = S, Se, Te$) monolayers via first-principles investigation

Hiep T. Nguyen, Nguyen Q. Cuong, Vo T. T. Vi,* Nguyen N. Hieu and Linh P. T. Tran

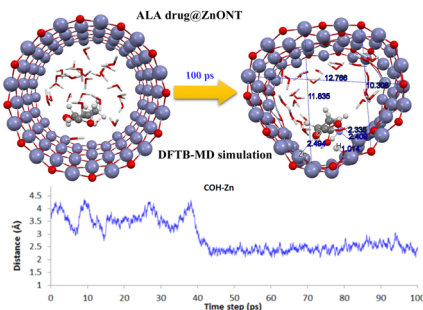
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Comprehensive study on the origin of orthorhombic phase stabilization in Gd-doped HfO_2 and DFT calculations

D. Banerjee,* C. C. Dey, Ravi Kumar, Brindaban Modak, Snehamoyee Hazra, Subarna Datta, Barnali Ghosh, S. V. Thakare, S. N. Jha and D. Bhattacharyya

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Toward functionalization of ZnO nanotubes and monolayers with 5-aminolevulinic acid drugs as possible nanocarriers for drug delivery: a DFT based molecular dynamic simulation

Masoumeh Mohammadzaheri, Saeed Jamehbozorgi,* Maosud Darvish Ganji, Mahyar Rezvani* and Zahra Javanshir

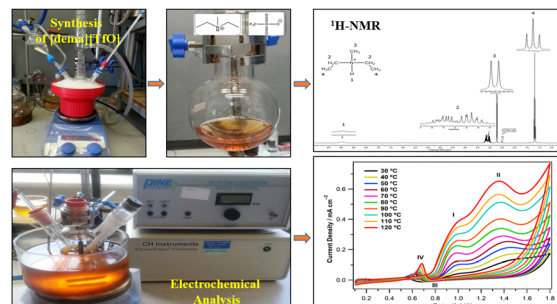


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Electrochemistry of ethanol and dimethyl ether at a Pt electrode in a protic ionic liquid: the electrode poisoning mechanism

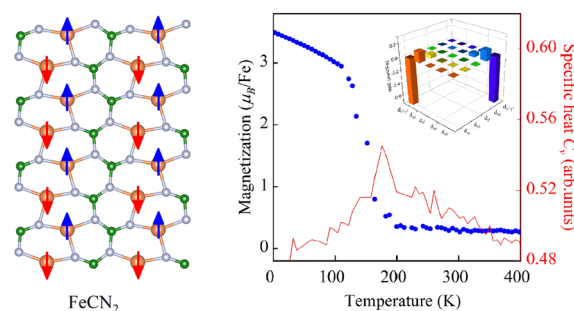
Sayyar Muhammad* and Darren Anthony Walsh



21521

An antiferromagnetic semiconducting FeCN₂ monolayer with a large magnetic anisotropy and strong magnetic coupling

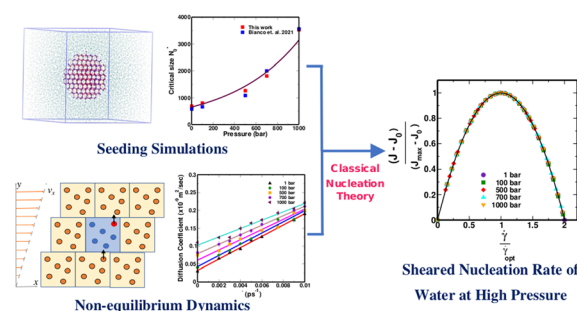
Zhicui Wang, Huan Lou, Fanjunjie Han, Xu Yan, Yong Liu* and Guochun Yang*



21528

Does supercooled water retain its universal nucleation behavior under shear at high pressure?

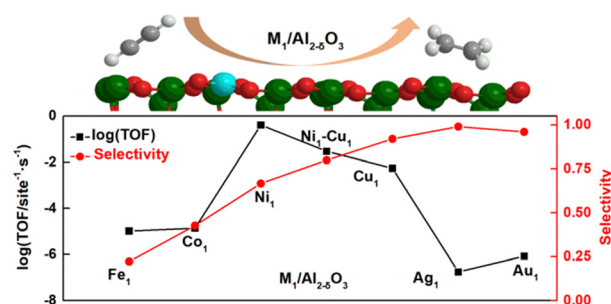
Snehitha Srirangam, Mangesh Bhendale and Jayant K. Singh*



21538

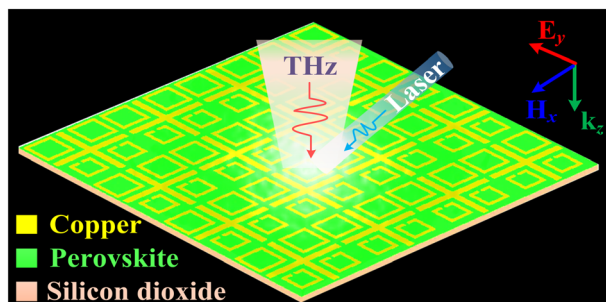
M supported on Al-defective Al_{2-δ}O₃ (M = Fe, Co, Ni, Cu, Ag, Au) as catalysts for acetylene semi-hydrogenation: a theoretical perspective

Bing-Bing Li, Hong-Yan Ma* and Gui-Chang Wang*



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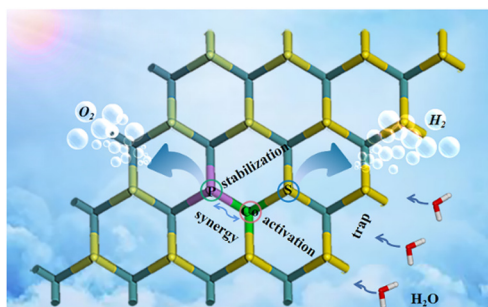
21547



High-transmission and large group delay terahertz triple-band electromagnetically induced transparency in a metal-perovskite hybrid metasurface

Mingming Chen* and Xue-Xia Yang*

21554



Enhancing photocatalytic overall water-splitting performance on dual-active-sites of the Co-P@MoS₂ catalysts: a DFT study

Jing Ma, Xin Wang,* Dongchun Yang, Jianhua Fan, Xiaoyong Lai, Roberts I. Eglitis and Yingtao Liu*

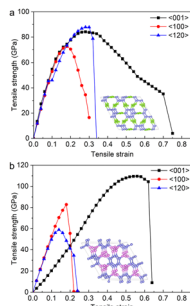
21562



Atomic autoionization in the photo-dissociation of super-excited deuterated water molecules fragmenting into D⁺ + O⁺ + D

W. Iskandar, T. N. Rescigno,* A. E. Orel, K. A. Larsen, B. Griffin, D. Call, V. Davis, B. Jochim, T. Severt, J. B. Williams, I. Ben-Itzhak, D. S. Slaughter and Th. Weber*

21573



Novel carbon allotropes in all-sp² bonding networks: self-assembling design and first-principles calculations

Ying Ma, Pan Ying,* Kun Luo, Yingju Wu, Baozhong Li, Qiaoyi Han and Julong He*

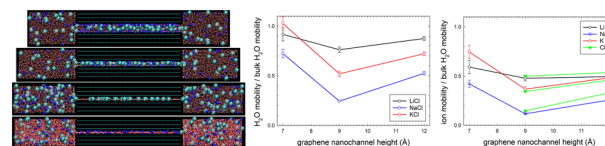


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21579

Structure and self-diffusivity of alkali-halide electrolytes in neutral and charged graphene nanochannels

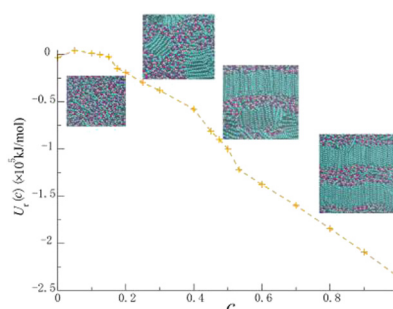
Eliška Rezlerová, Filip Moučka, Milan Předota and Martin Lisal*



21595

Phase coexistence in $[C_{22}/C_{1}MIm]^+ [NO_3]^-$ ionic-liquid mixtures and first-order phase transitions from homogeneous liquid to smectic B by varying the cation ratio

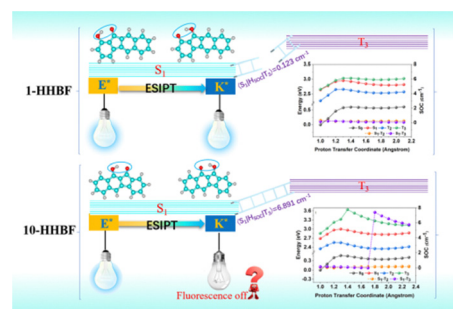
Jie Yao, Giacomo Saielli, Fanlong Meng and Yanting Wang*



21604

ESIPT-induced spin-orbit coupling enhancement leads to tautomer fluorescence quenching of the 10-HHBF molecule

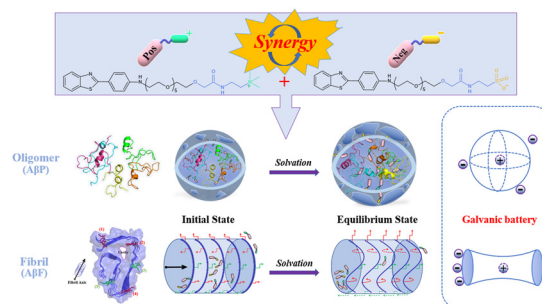
Xin Zhao, Hang Yin,* Wentian Zhang, Jie Guo and Ying Shi*



21612

Origin of stronger binding of ionic pair (IP) inhibitor to Aβ42 than the equimolar neutral counterparts: synergy mechanism of IP in disrupting Aβ42 protofibril and inhibiting Aβ42 aggregation under two pH conditions

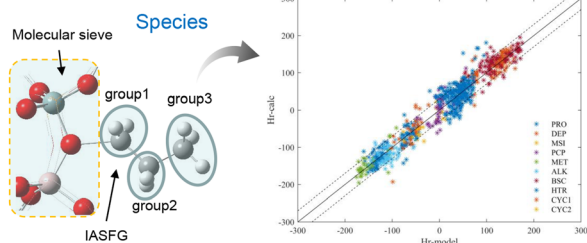
Wen Xu, Jinfei Mei, Chuanbo Wang, Huijuan Yang, Xiaohong Ma, Wenqi Gao, Sajjad Ahmad and Hongqi Ai*



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21631

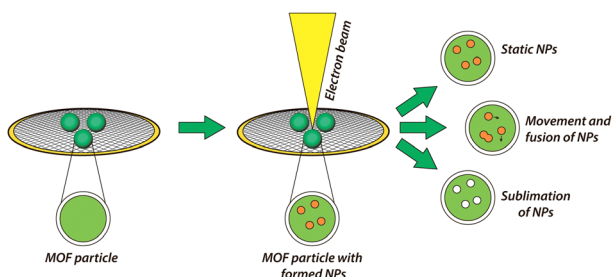
$$Y_f = \sum_{i=1}^{n_c} n_{g_i} \cdot g_{c_i} + y_{MS} + y_{MOL}$$



A modified group contribution method for estimating thermodynamic parameters of methanol-to-olefins over a SAPO-34 catalyst

Junyi Yu, Hua Li,* Mao Ye* and Zhongmin Liu

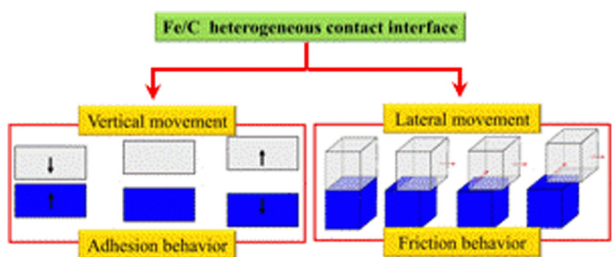
21640



Dynamic behavior of metal nanoparticles in MOF materials: analysis with electron microscopy and deep learning

Kirill S. Erokhin, Evgeniy O. Pentsak, Vyacheslav R. Sorokin, Yury V. Agaev, Roman G. Zaytsev, Vera I. Isaeva and Valentine P. Ananikov*

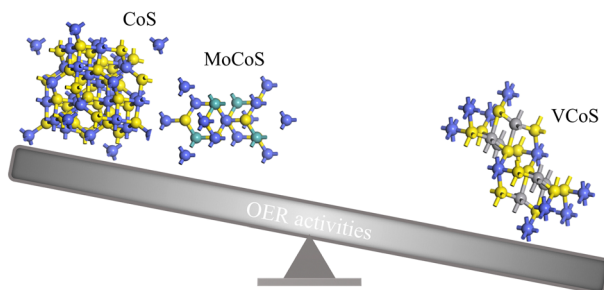
21649



Adhesion and friction behaviors of a γ -Fe/diamond heterogeneous contact interface: a density functional theory study

Qizhen He, Lixiang Rao,* Wenwei Song, Hailiang Liu, Silong Zhang, Xuejun Ren and Qingxiang Yang*

21661



Experimentally revealed and theoretically certified synergistic electronic interaction of V-doped CoS for facilitating the oxygen evolution reaction

Jingjing Zhang, Wei Deng,* Yun Weng, Xiang Li, Haifang Mao,* Tiandong Lu, Wenqian Zhang, Dewu Long and Fei Jiang*

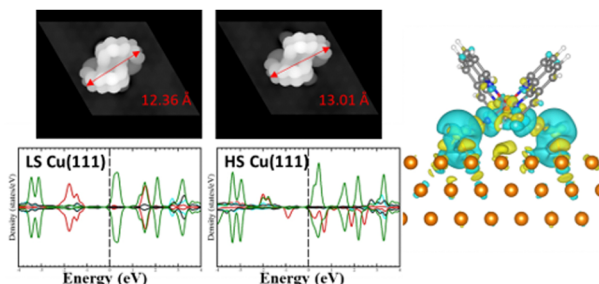


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21673

How complex–surface interactions modulate the spin transition of Fe(II) SCO complexes supported on metallic surfaces?

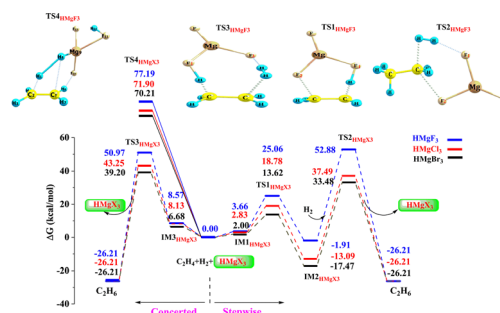
Rocío Sánchez-de-Armas,* Iman Jaber El lala and Carmen J. Calzado



21684

Unveiling the correlation between the catalytic efficiency and acidity of a metal-free catalyst in a hydrogenation reaction. A theoretical case study of the hydrogenation of ethene catalyzed by a superacid arising from a superhalogen

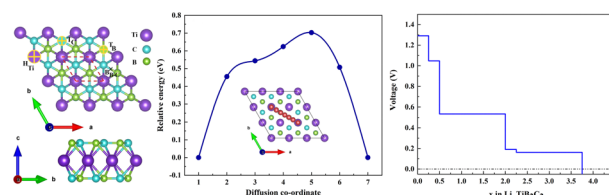
Jin-Feng Li,* Lan Luo, Zhi-Hui Bai and Bing Yin*



21699

Two-dimensional Dirac TiB₂C₂ as a potential anode material for Li-ion batteries: a first-principles study

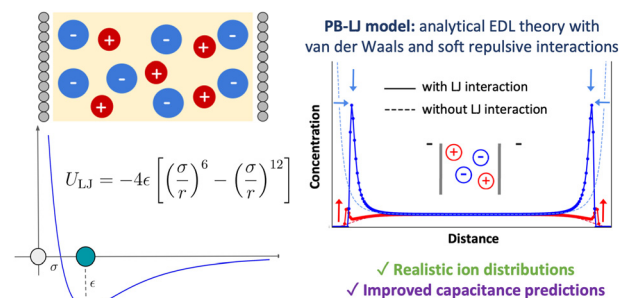
A. Etrini,* A. Elomrani, S. Oukahou, M. Maymoun, K. Sbiaai and A. Hasnaoui*



21708

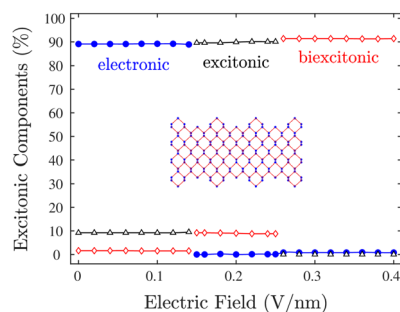
Incorporating ion-specific van der Waals and soft repulsive interactions in the Poisson–Boltzmann theory of electrical double layers

Aniruddha Seal, Utkarsh Tiwari, Ankur Gupta and Ananth Govind Rajan*



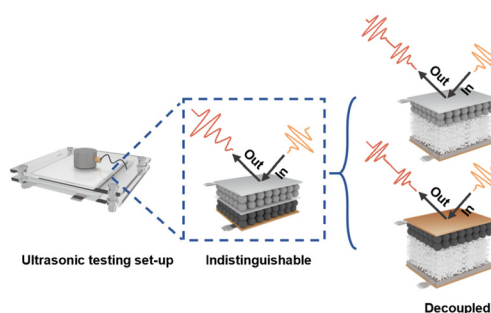
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21723

**Excitonic ground states in phosphorene nanoflakes**

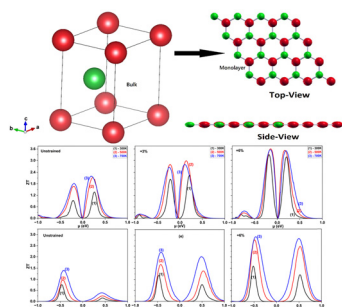
Jun Zhong, Wenzhuo Huang and Weidong Sheng*

21730

**Decoupling of the anode and cathode ultrasonic responses to the state of charge of a lithium-ion battery**

Xueting Liu, Zhe Deng, Yaqi Liao, Jinqiao Du, Jie Tian, Zijun Liu, Yue Shen* and Yunhui Huang*

21736

**Intrinsic and strain dependent ultralow thermal conductivity in novel AuX (X = Cu, Ag) monolayers for outstanding thermoelectric applications**Aadil Fayaz Wani, Shakeel Ahmad Khandy,*
Lokanath Patra, Marutheeswaran Srinivasan, Jaspal Singh,
Atif Mossad Ali, Ishtihadah Islam, Shobhna Dhiman and
Kulwinder Kaur*