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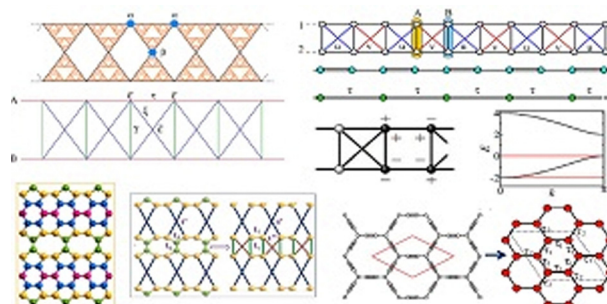
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REVIEW

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Application of the real space decimation method in determining intricate electronic phases of matter: a review

Amrita Mukherjee, Arka Bandyopadhyay and
Debnarayan Jana*

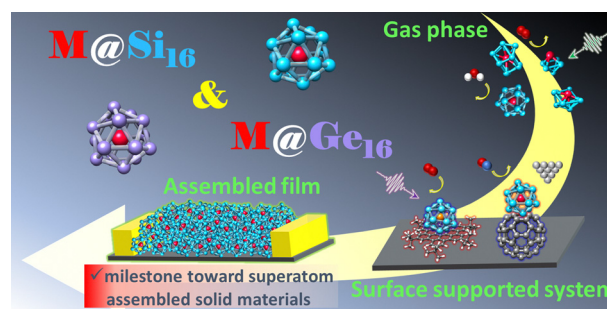


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Bridging the gas and condensed phases for metal-atom encapsulating silicon- and germanium-cage superatoms: electrical properties of assembled superatoms

Takaho Yokoyama and Atsushi Nakajima*



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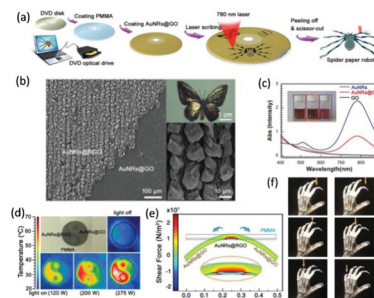


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Laser defined and driven bio-inspired soft robots toward complex motion control

Monan Liu, Qing Wang, Ai-Wu Li* and Hong-Bo Sun

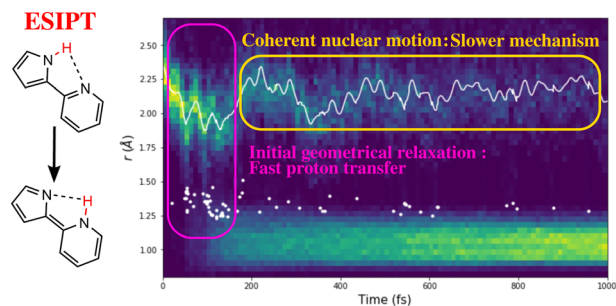


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ESIPT in the pyrrol pyridine molecule: mechanism, timescale and yield revealed using dynamics simulations

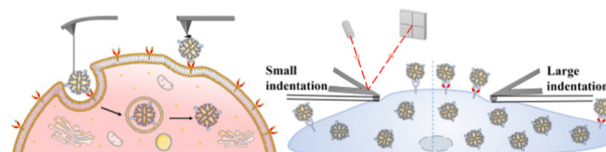
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Investigating the trans-membrane transport of HAIYPRH peptide-decorated nano-drugs

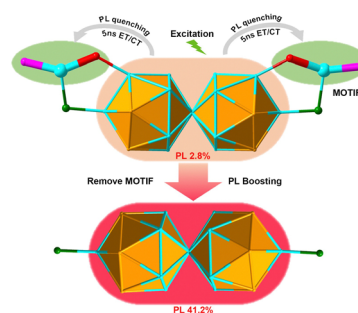
Xiaowan Zhang, Meirong Shan, Siying Li, Jing Zhao, Xuelei Pang, Guocheng Yang and Yuping Shan*



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Au₁₀Ag₁₇(TPP)₁₀(SR)₆Cl₅ nanocluster: structure, transformation and the origin of its photoluminescence

Along Ma, Jiawei Wang, Jie Kong, Yonggang Ren, Yuxuan Wang, Xiaoshuang Ma, Meng Zhou* and Shuxin Wang*

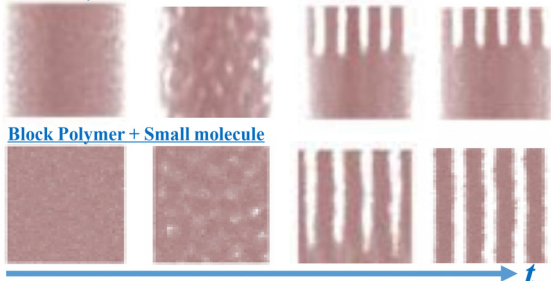


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Block Polymer

Block Polymer + Small molecule

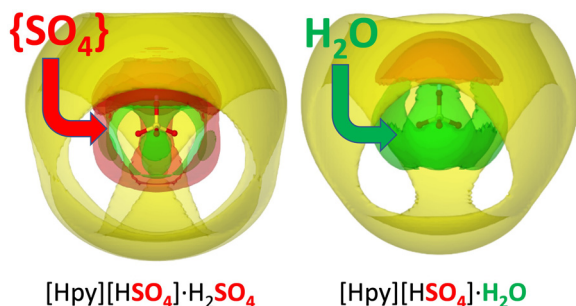


Catalytic assembly of symmetric diblock copolymers in a thin film: a dissipative particle dynamics simulation study

Tongwei Chen, Yunhan Zhang,* Shiyao Xiao, Dongbao Yao, Wei Jiang* and Haojun Liang*

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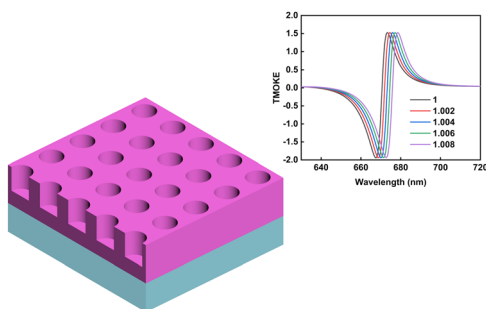
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The structure of protic ionic liquids based on sulfuric acid, doped with excess of sulfuric acid or with water

Anne McGrogan, Emily L. Byrne, Robert Guiney, Thomas F. Headen, Tristan G. A. Youngs, Anna Chrobok, John D. Holbrey* and Małgorzata Swadźba-Kwaśny*

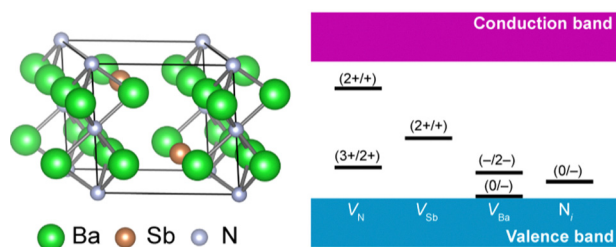
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Enhanced transverse magneto-optical Kerr effect using ferromagnetic metal perforated with nanopore arrays

Weiwei Zhang,* Guoqiang Du, Hongming Chen and Kang An*

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Defect-tolerant antiperovskite Ba_3SbN Native point defects in antiperovskite Ba_3SbN : a promising semiconductor for photovoltaics

Youngho Kang

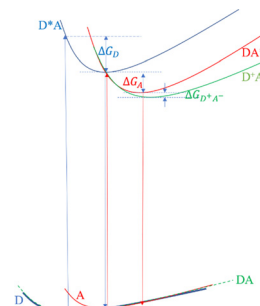


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Physical mechanisms on FRET and ICT for efficient Y6:PM6 as bulk heterojunction active layers

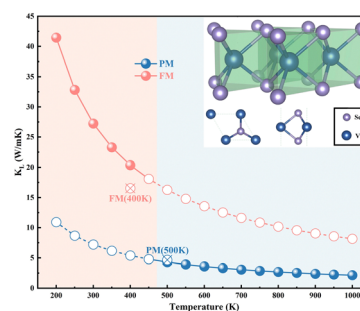
Wenwen Li, Jing Li and Mengtao Sun*



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The effect of magnetic order on the thermal transport properties of the intrinsic two-dimensional magnet 2H-VSe₂

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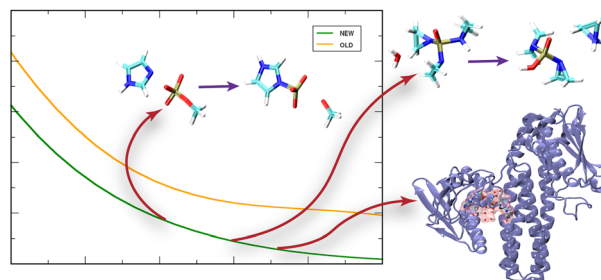


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Extended-sampling QM/MM simulation of biochemical reactions involving P–N bonds

Mayukh Kansari, Lena Eichinger and Tomáš Kubař*

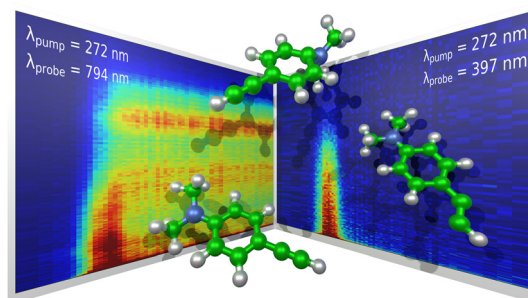
Nitrogen phosphorylation in proteins simulated with a new parametrization of DFTB3



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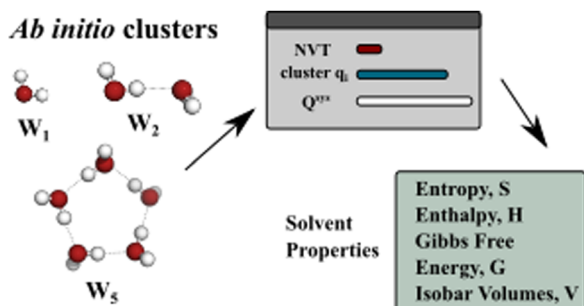
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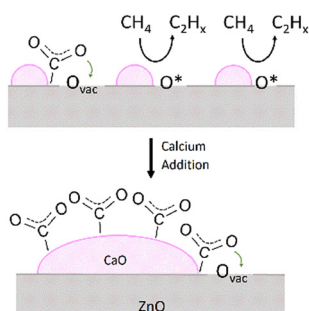
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Appropriate cluster set selection for the prediction of thermodynamic properties of liquid water with QCE theory

Fairuz H. Hashim, Fiona Yu and Ekaterina I. Izgorodina*

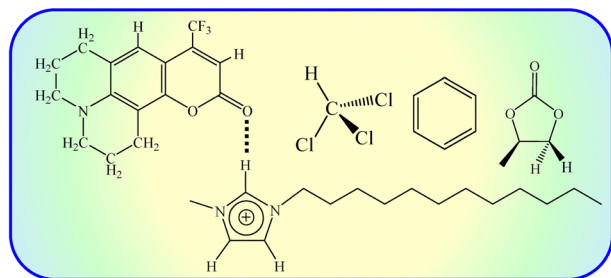
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Surface basicity controls C–C coupling rates during carbon dioxide-assisted methane coupling over bifunctional Ca/ZnO catalysts

Leah R. Filardi, Feipeng Yang, Jinghua Guo, Coleman X. Kronawitter* and Ron C. Runnebaum*

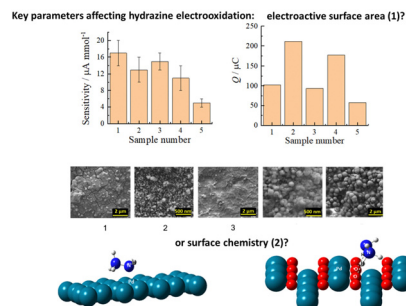
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Solvation structure and dynamics of coumarin 153 in an imidazolium-based ionic liquid with chloroform, benzene, and propylene carbonate

Toshiyuki Takamuku,* Daiki Nishiyama, Masahiro Kawano, François-Alexandre Miannay and Abdenacer Idrissi

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First principles of hydrazine electrooxidation at oxide-free and oxide-based palladium electrodes in complex media

E. V. Zolotukhina, E. V. Butyrskaya, M. Koch, P. Herbeck-Engel, M. G. Levchenko and Y. E. Silina*

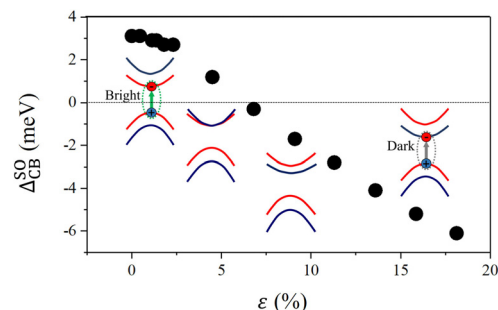


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Strain-induced dark exciton generation in rippled monolayer MoS₂

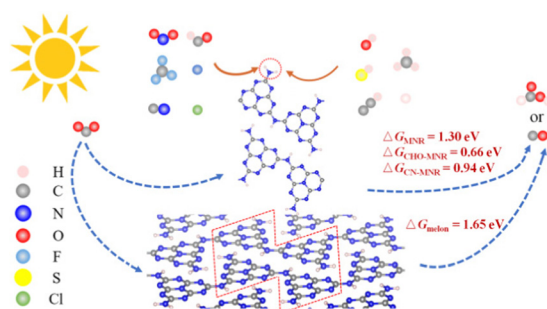
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Materials design of edge-modified polymeric carbon nitride nanoribbons for the photocatalytic CO₂ reduction reaction

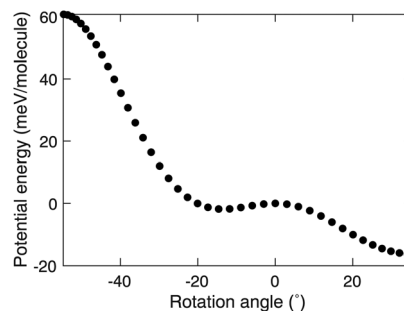
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Unique features of the structural phase transition in acetylene showing simultaneous characteristics of reconstructive, displacive and order–disorder

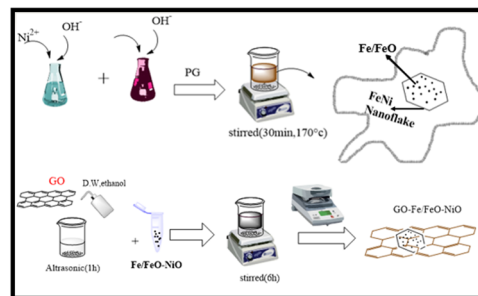
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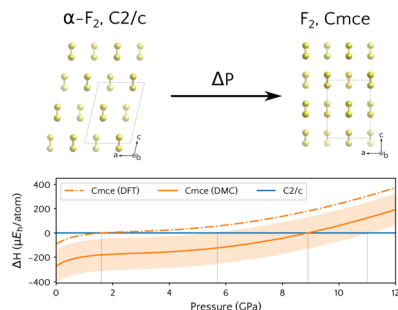
Microwave absorption property of GO–Fe/FeO–NiO HNFs: GO decorated Fe/FeO–NiO hexagonal flakes with a 2D/0D/2D structure

Mozhgan Arabi, Seyyed Mahdy Baizaei* and Hoda Hekmatara*



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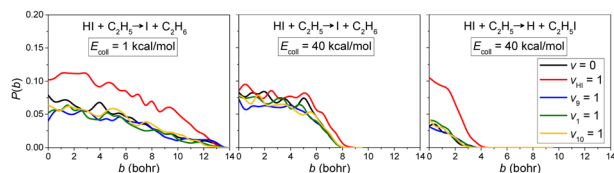
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Pressure-induced second-order phase transition in fluorine

Giovani L. Rech,* André L. Martinotto, Janete E. Zorzi and Cláudio A. Perottoni

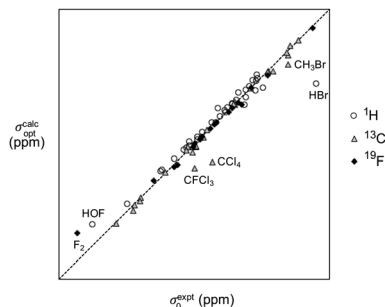
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Vibrational mode-specific quasi-classical trajectory studies for the two-channel HI + C₂H₂ reaction

Cangtao Yin* and Gábor Czakó*

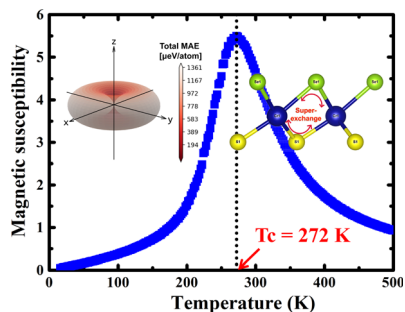
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Simple, accurate, adjustable-parameter-free prediction of NMR shifts for molecules in solution

Emlyn M. Hoyt, Lachlan O. Smith and Deborah L. Crittenden*

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High temperature ferromagnetic metal: a Janus CrS₂Se monolayer

Yaxuan Wu, Qingquan Liu, Puyuan Shi, Jingjuan Su, Yungeng Zhang* and Bing Wang*

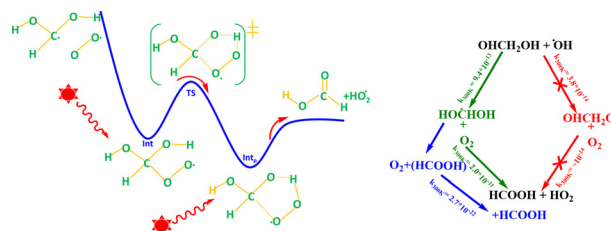


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Effect of formic acid on $O_2 + OH^*CHOH \rightarrow HCOOH + HO_2$ reaction under tropospheric condition: kinetics of *cis* and *trans* isomers

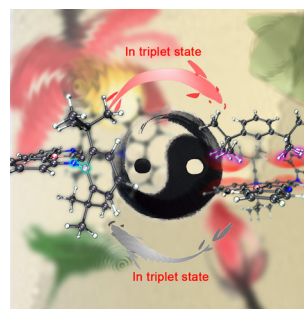
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Dynamic stability of a blue multi-resonance thermally activated delayed fluorescence molecule without damaging the luminescence properties

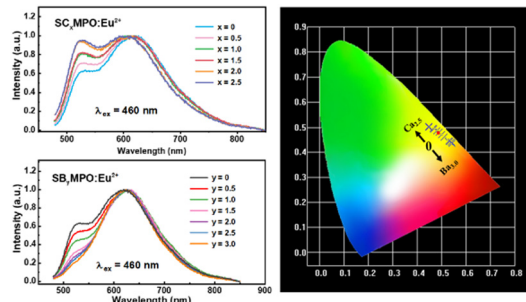
Heming Zhang,* Lianbao Ke, Yufang Nie, Jiaxuan Wang and Hai Bi*



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Site-selective occupation, optical spectrum regulation and photoluminescence property investigation of Eu^{2+} -activated blue light-excited yellow-orange emitting phosphors

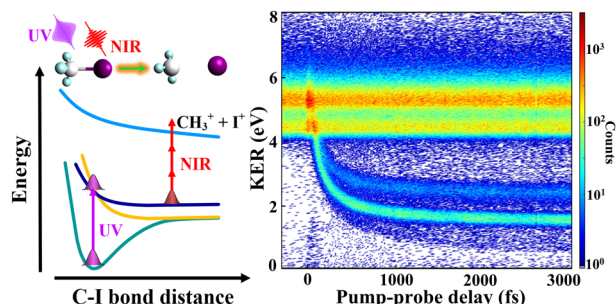
Wenzhi Sun,* Tingting Zhao, Shuya Wang, Denghu Wei, Mengmeng Jiao and Hongwu Zhang*



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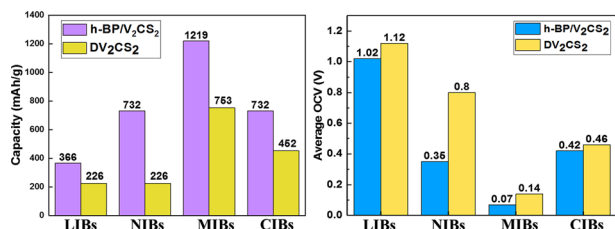
Single- and multi-photon-induced ultraviolet excitation and photodissociation of CH_3I probed by coincident ion momentum imaging

Farzaneh Ziaee, Kurtis Borne, Ruaidh Forbes, Kanaka Raju P., Yubaraj Malakar, Balram Kaderiya, Travis Severt, Itzik Ben-Itzhak, Artem Rudenko* and Daniel Rolles*



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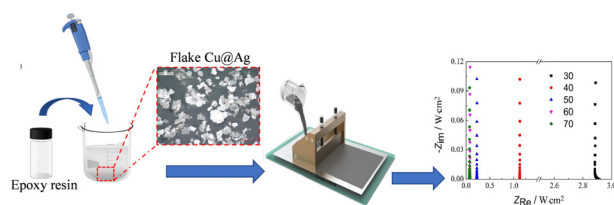
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Comparative studies of hexagonal boron phosphide/V₂CS₂ heterostructure and homogeneous bilayers as metal-ion battery anodes

Xian Yuan, Zhongyong Zhang, Yuping He and Naigen Zhou*

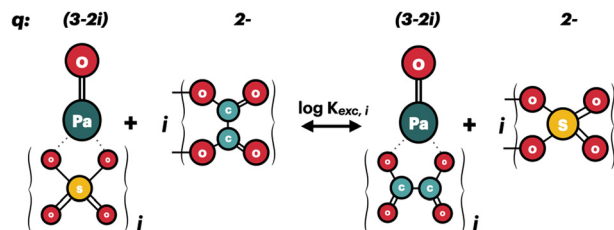
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Effect of flake silver-plated copper particles on the property enhancement of electrically conductive adhesives

Na Cheng, Zhi Sun, Xiaohui Yu,* Qianzhen Yu and Jianwei Zhao*

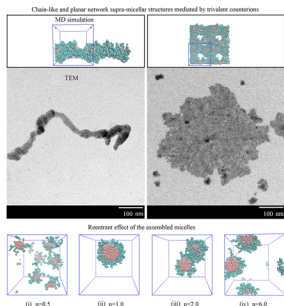
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Coordination and thermodynamic properties of aqueous protactinium(v) by first-principle calculations

Hanna Oher, Jérémy Delafoulhouze, Eric Renault, Valérie Vallet and Rémi Maurice*

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Self-assembly of amphiphilic polyelectrolytes in trivalent salt solution

Liyan Liu,* Fujia Wang, Xinyi Liu, Lide Guo, Xiujuan Gao and Hongge Tan*

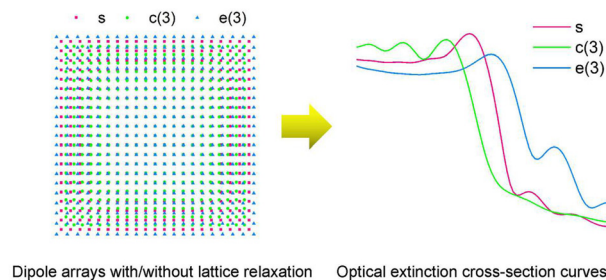


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Lattice relaxation effects on the collective resonance spectra of a finite dipole array

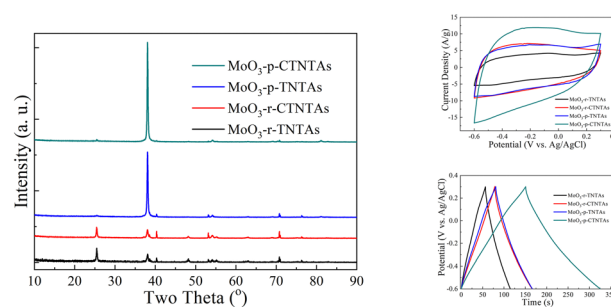
Baodong Gai,* Jingwei Guo and Yuqi Jin



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Supercapacitive performance of C-axis preferentially oriented TiO₂ nanotube arrays decorated with MoO₃ nanoparticles

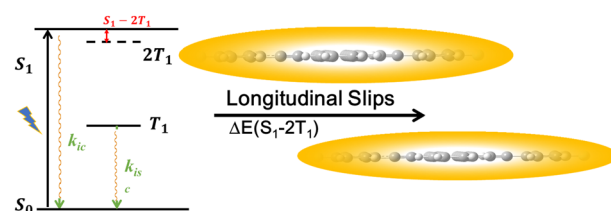
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Design of BPEA-based derivatives with high singlet fission performance: a theoretical perspective

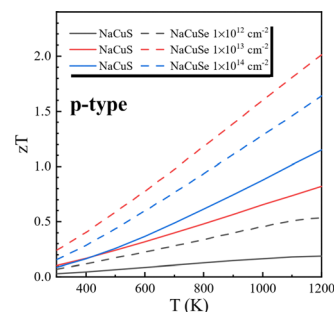
Jian Song,* Hongjin Li, Zhongpo Zhou, Yonggang Yang,* ChaoChao Qin and Yufang Liu



10082

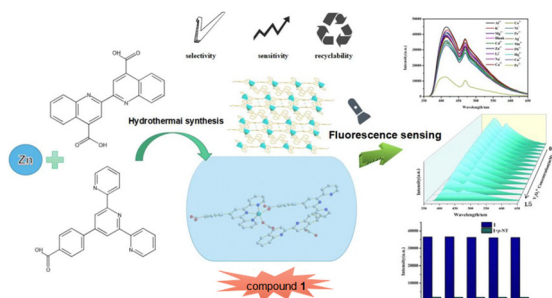
Thermoelectric response of single quintuple layer sodium copper chalcogenides persisting at high temperature

Yuhong Huang, Xuanhong Zhong, Zhu Yu Feng, Shujing Lin, Hongkuan Yuan and Hong Chen*



RESEARCH PAPERS

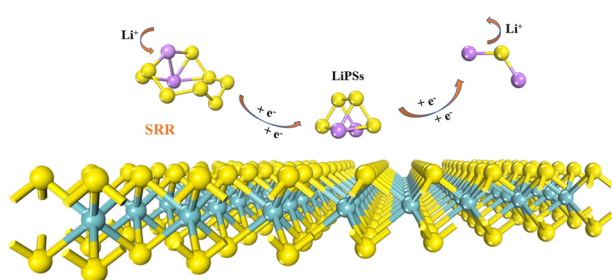
10090



A Zn-coordination polymer as a multifunctional fluorescent probe for the detection of $V_2O_7^{4-}$, Fe^{3+} , and *p*-nitrotoluene

Shengsheng Qi, Zhang Li, Yuejiao Jia, Dechao Li and Ming Hu*

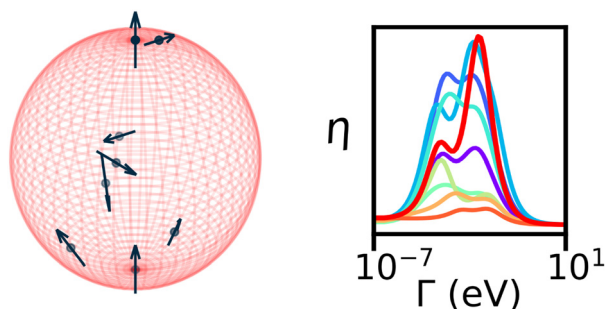
10097



A theoretical study of the NbS_2 monolayer as a promising anchoring material for lithium–sulfur batteries

Xinxin Zhang, Xiaocheng Zhou,* Yu Wang and Yafei Li*

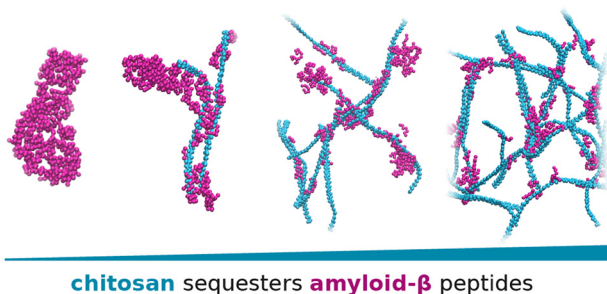
10103



From Goldilocks to twin peaks: multiple optimal regimes for quantum transport in disordered networks

Alexandre R. Coates, Brendon W. Lovett and Erik M. Gauger*

10113



Mechanistic insights into the inhibition of amyloid- β aggregation by chitosan

Suhas Gotla and Silvina Matysiak*

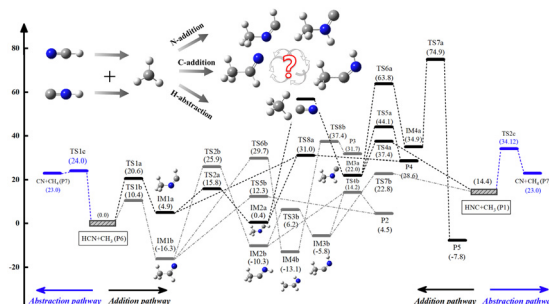


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10121

Theoretical study on the kinetics of hydrogen cyanide and hydrogen isocyanide reactions with the methyl radical

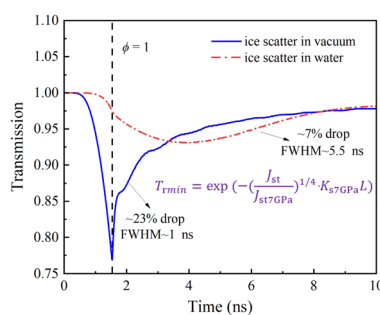
Jibiao Xie and Jinou Song*



10129

Insights into water freezing from classical nucleation theory

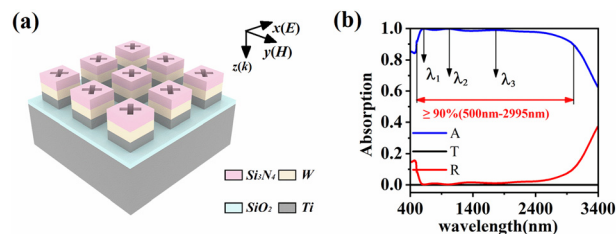
Xichen Huang, Yanyun Sun,* Xiaoxi Tan, Chaobo Zhang, Yu Huang, WenQiang Liao and Fusheng Liu



10136

Metamaterial ultra-wideband solar absorbers based on a multi-layer structure with cross etching

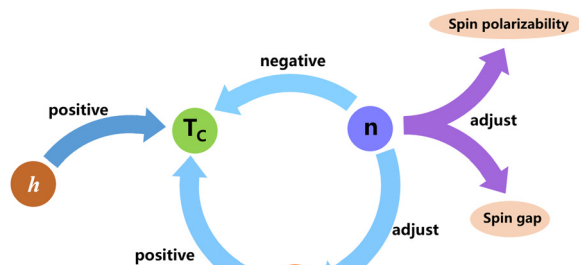
Pengfei Sun, Hengli Feng, Lijing Su, Sihan Nie, Xin Li, Yaxin Zhou, Lingling Ran and Yang Gao*



10143

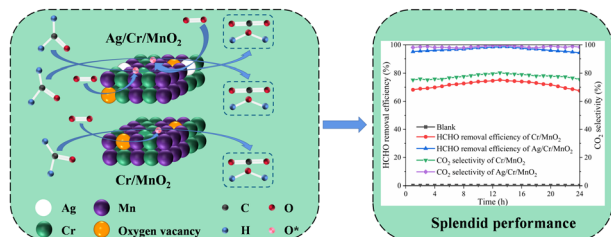
Ferromagnetic vanadium disulfide VS₂ monolayers with high Curie temperature and high spin polarization

Hao-Jia Wu, Yu-Lu Wan, Zhao-Yi Zeng, Cui-E Hu,* Xiang-Rong Chen* and Hua-Yun Geng



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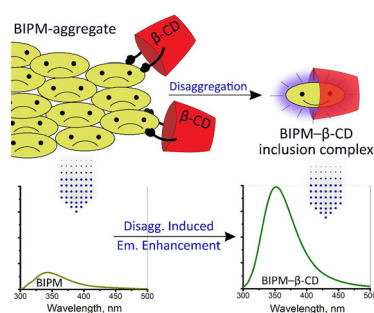
10155



Ag-promoted Cr/MnO₂ catalyst for catalytic oxidation of low-concentration formaldehyde at room temperature

Chaomin Duan, Mianwu Meng,* Huang Huang,* Heng Wang,* Hua Ding and Qi Zhang

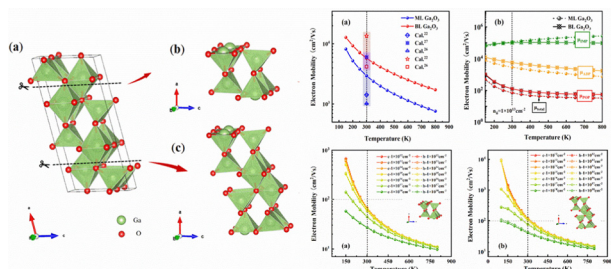
10166



Disaggregation-induced resurgence of quenched emission of a self-assembled bis-indole system: photophysics, energetics, and dynamics

Provakar Paul, Saikat Samanta, Arunavo Chatterjee, Arabinda Mallick* and Tapas Majumdar*

10175



Nontrivial role of polar optical phonons in limiting electron mobility of two-dimensional Ga₂O₃ from first-principles

Xinlei Duan, Tianyu Wang, Zhiwei Fu, Linhua Liu* and Jia-Yue Yang*

CORRECTIONS

10184

Correction: 5D total scattering computed tomography reveals the full reaction mechanism of a bismuth vanadate lithium ion battery anode

Jonas Sottmann, Amund Ruud, Øystein S. Fjellvåg, Gavin B. M. Vaughan, Marco Di Michel, Helmer Fjellvåg, Oleg I. Lebedev, Ponniah Vajeeston and David S. Wragg*



CORRECTIONS

10185

Correction: Atmospheric chemistry of (Z)- and (E)-1,2-dichloroethene: kinetics and mechanisms of the reactions with Cl atoms, OH radicals, and O₃

Mads P. Sulbaek Andersen,* Aleksandra Volkova, Sofie A. Hass, Jonathan W. Lengkong, Dvian Hovanesian, Theis I. Sølling, Timothy J. Wallington and Ole J. Nielsen

10186

Correction: Atmospheric chemistry of CF₃CN: kinetics and products of reaction with OH radicals, Cl atoms and O₃

Mads Peter Sulbaek Andersen,* Joanna Ohide, Theis I. Sølling and Ole John Nielsen

