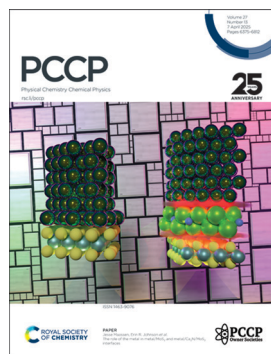


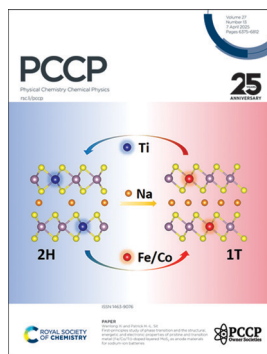
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See Jesse Maassen, Erin R. Johnson *et al.*, pp. 6438–6446. Image reproduced by permission of Adrian F. Rumson from *Phys. Chem. Chem. Phys.*, 2025, 27, 6438.



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See Wenlong Xi and Patrick H.-L. Sit, pp. 6447–6456. Image reproduced by permission of Wenlong Xi and Patrick H.-L. Sit from *Phys. Chem. Chem. Phys.*, 2025, 27, 6447.

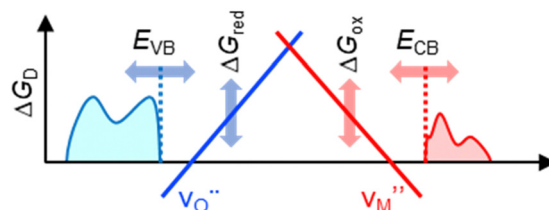
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The physics of defect chemistry and the chemistry of defect physics

Andreas Klein* and Denis Sudarikov

$$\Delta G_{\text{red}} = \Delta G_{vO^{\bullet\bullet}}(\mu_O = 0, E_F = E_{CB}) + \frac{1}{2} \mu^0(O_2)$$

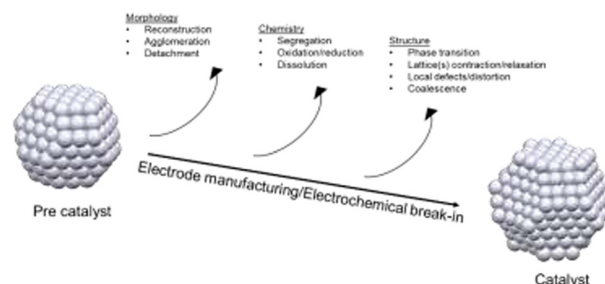


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Carlos A. Campos-Roldán,* Raphaël Chattot, Pierre-Yves Blanchard, Deborah J. Jones and Sara Cavaliere*



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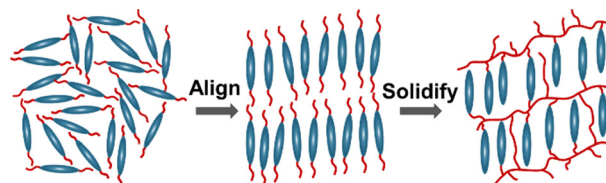
Fundamental questions
Elemental answers

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Liquid crystals as solid-state templates

Nurjahan Khatun, Agnes C. Nkele and Kushal Bagchi*

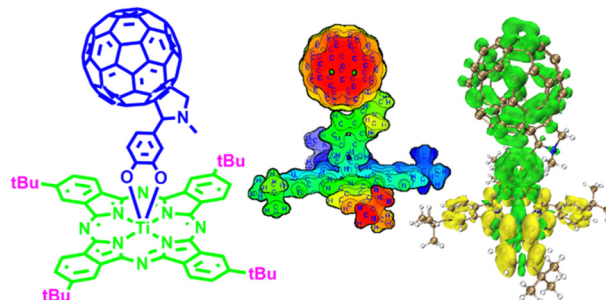


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The role of peripheral F-/H-atoms and *tert*-butyl substituents in charge transfer of axially substituted titanium phthalocyanines

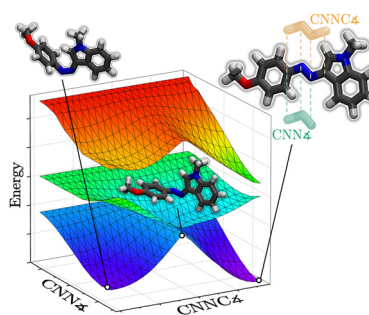
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Allen H. Chen, Zachary J. Knepp, Christian A. Guzman, Elizabeth R. Young* and Lisa A. Fredin*

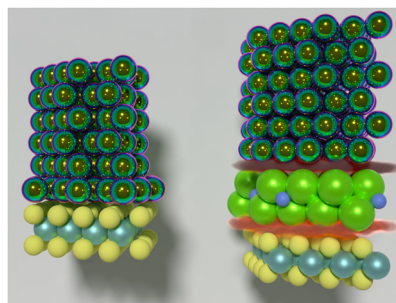


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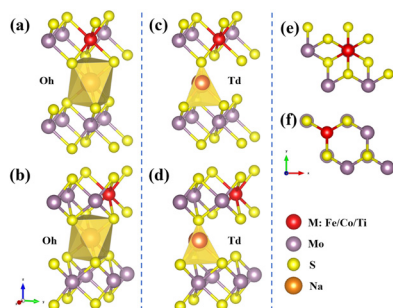
The role of the metal in metal/MoS₂ and metal/Ca₂N/MoS₂ interfaces

Adrian F. Rumson, Mohammad Rafiee Diznab, Jesse Maassen* and Erin R. Johnson*



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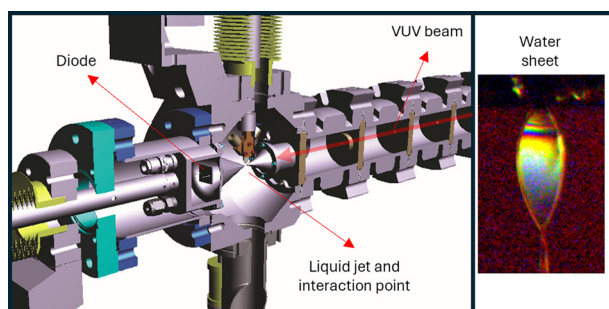
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First-principles study of phase transition and the structural, energetic and electronic properties of pristine and transition metal (Fe/Co/Ti)-doped layered MoS_2 as anode materials for sodium-ion batteries

Wenlong Xi and Patrick H.-L. Sit*

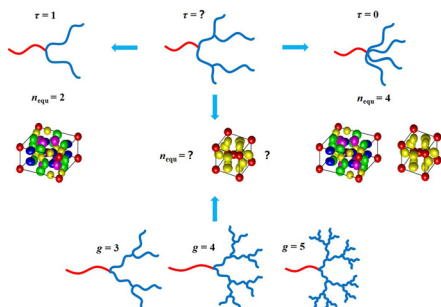
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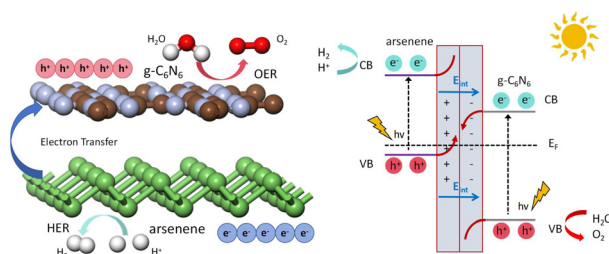
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Jiahao Shi, Qingshu Dong,* Tao Yang and Weihua Li*

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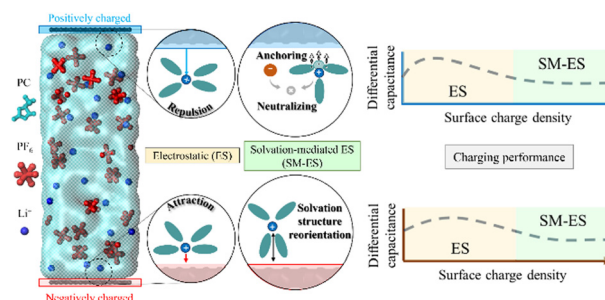


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Solvation-mediated adsorption mechanism of solvated lithium ions at a charged solid–liquid interface for electrochemical energy storage: atomic scale investigation and insights

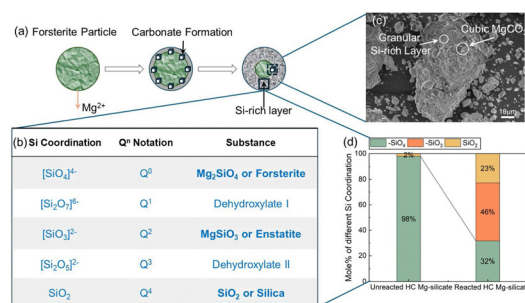
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Evolution of silicate coordination in architected amorphous and crystalline magnesium silicates during carbon mineralization

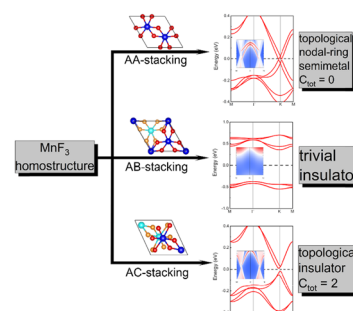
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Stacking induced symmetry breaking and gap opening in Dirac half-metal MnF₃

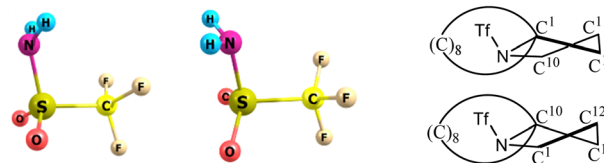
Wentai Xiang and Baozeng Zhou*



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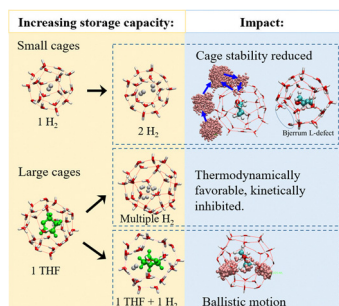
Gas-phase *versus* crystal structure of triflamide and some of its heterocyclic derivatives

Bagrat A. Shainyan,* Alexey V. Eroshin and Sergey A. Shlykov*



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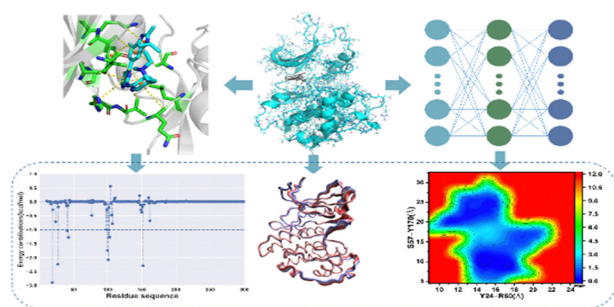
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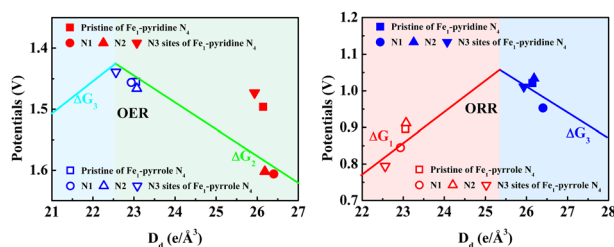
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Insights into phosphorylation-induced influences on conformations and inhibitor binding of CDK6 through GaMD trajectory-based deep learning

Lu Zhao,* Jian Wang, Wanchun Yang, Canqing Zhang, Weiwei Zhang and Jianzhong Chen*

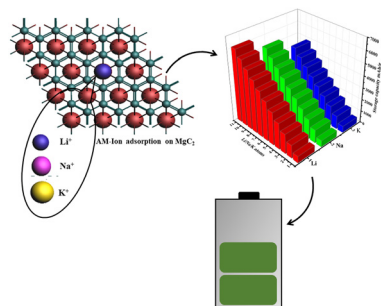
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Tailoring OER/ORR activity in TM₁N₄ catalysts through first-/second-shell nitrogen doping: a density functional theory investigation

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A DFT study of monolayer magnesium carbide (MgC₂) as a potential anode for (Li, Na, K) alkali metal-ion batteries

Muhammad Akbar, Noor ul Ain, Muhammad Isa Khan,* Rajeh Alotaibi, Syed Mansoor Ali and Naveed Ashraf

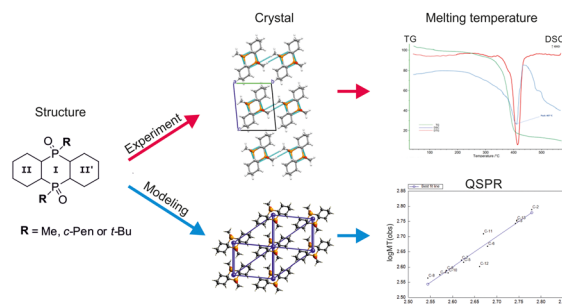


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Rationalization of the thermal properties of some polycyclic organophosphorus compounds by structural and QSPR analyses

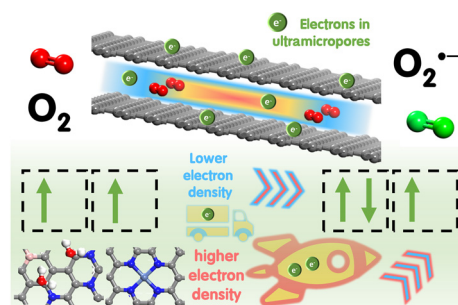
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Increasing the local electron density of carbons for enhanced O₂ activation at room temperature

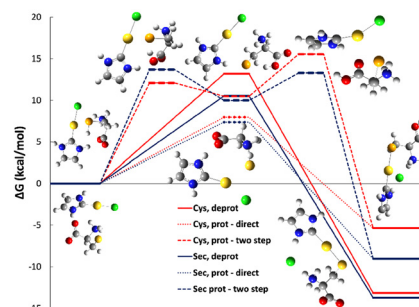
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pH control of the reaction mechanism: interactions of the Au(I)-NHC complex with thioredoxin reductase (modeled by cysteine and selenocysteine); *ab initio* and DFT calculations

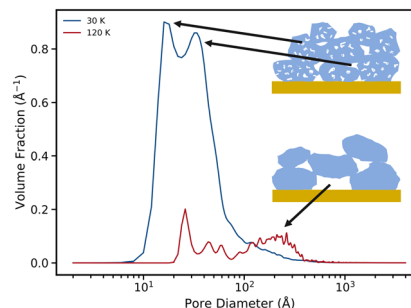
Filip Šebesta, Man Thi Hong Nguen, Markéta Munzarová and Jaroslav V. Burda*



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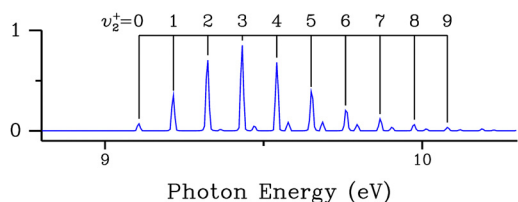
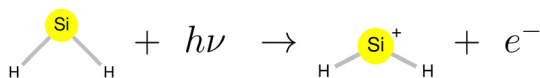
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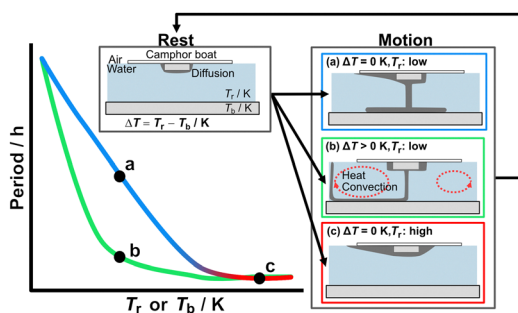
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The threshold-photoelectron spectrum of SiH₂: experiment and modeling with MCTDH method

L. H. Coudert,* N. L. Chen, B. Gans, S. Boyé-Péronne, G. A. Garcia, S. Hartweg and J.-C. Loison

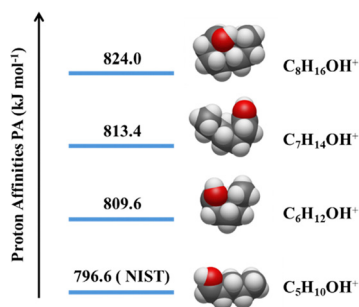
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Oscillatory motion of a self-propelled object determined by the mass transport path

Masakazu Kuze, Nozomi Kawai, Muneyuki Matsuo,* Istvan Lagzi, Nobuhiko J. Suematsu and Satoshi Nakata*

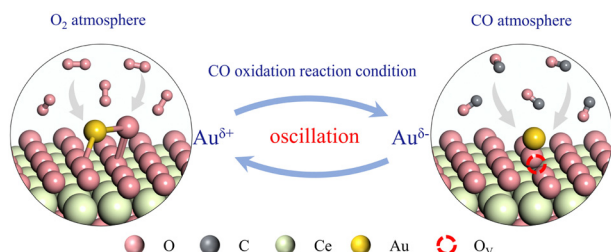
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Proton affinities of aldehyde molecules determined from the forward and backward gas-phase proton transfer reactions in a selected ion flow-drift tube

Maroua Omezzine Gnioua, Anatolii Spesyvyi and Patrik Španěl*

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An environmentally adaptive gold single-atom catalyst with variable valence states

Meiliang Ma, Wen Liu, Xiaojuan Hu,* Ying Jiang, Wentao Yuan, Zhong-Kang Han* and Yong Wang

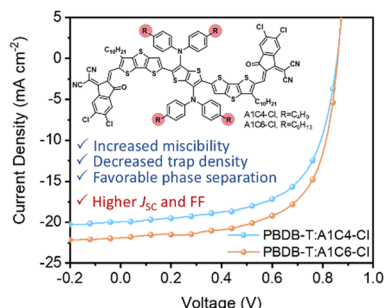


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Optimizing the miscibility for enhanced photovoltaic performance of non-fused ring electron acceptors through side-chain engineering

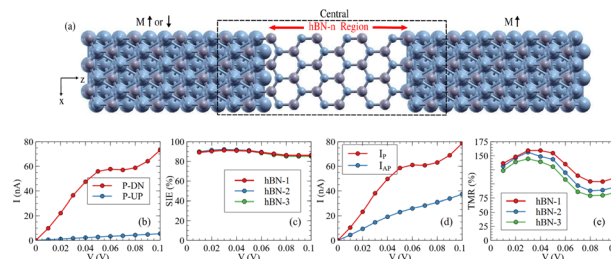
Yahui Bai, Linwei Xie, Zhihui Lin, Qi Ai, Fuwen Zhao and Dan He*



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An *Ab initio* study on the enhancement of tunneling magnetoresistance and spin injection in Ni/vacuum/Ni magnetic tunnel junctions by h-BN stacking

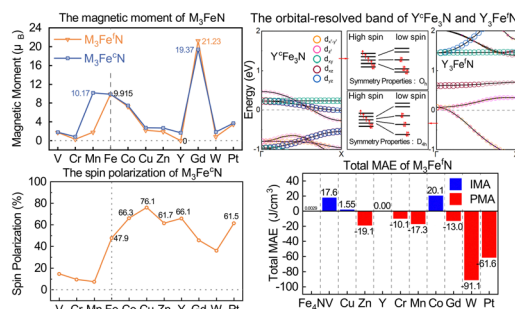
Ziqi Han, Chun-Sheng Liu, Xiaohong Zheng,* Da-Yong Liu,* Weiyang Wang* and Yushen Liu



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The emergence of novel magnetic properties in ternary iron nitrides toward spintronics: first-principles calculations

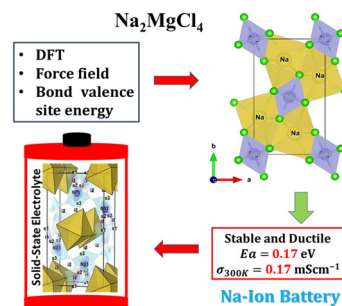
Ke Xiao, Xiaohui Shi,* Xingyuan Zhang, Qingming Ping and Lulu Du*



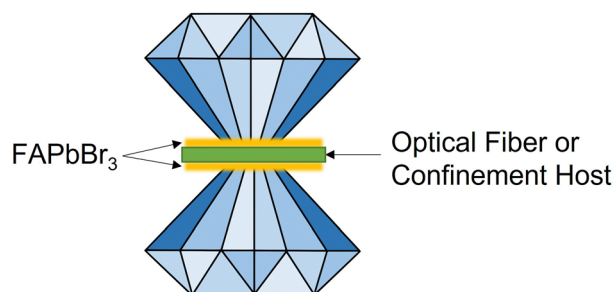
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Theoretical evaluation of Na₂MgCl₄ double chlorite as an electrolyte for all-solid-state sodium-ion batteries

Yohandys A. Zulueta, Jose R. Fernández-Gamboa, Narciso Antonio Villar Goris, My Phuong Pham-Ho and Minh Tho Nguyen*



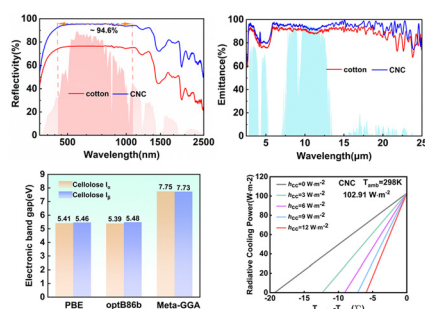
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Enhanced structural stability of formamidinium lead bromide (FAPbBr₃) perovskites in confined and coated configurations under varying pressures

Hai Yen Thi Nguyen, Duc Huy Nguyen, Chien-Chih Lai,*
Christopher M. Burba,* Yuan-Cheng Chung and
Hai-Chou Chang*

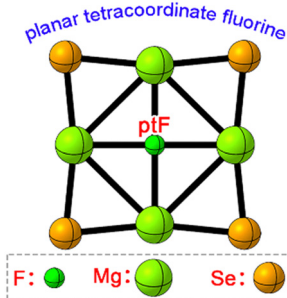
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Physical insights into the high radiative cooling power of cellulose-based materials

Zhuo Zhao, Jian Zhang, Yuan Cheng, Aijun Hou,
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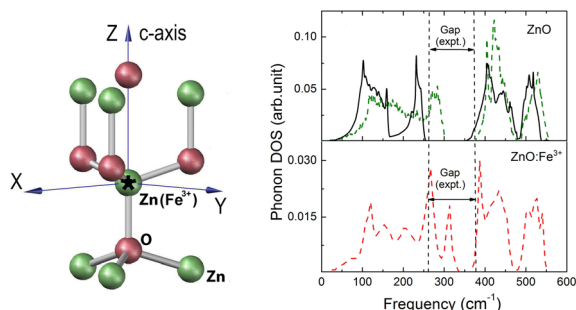
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Planar tetracoordinate fluorine in a FMg₄Se₄⁻ cluster

Rui Sun, Caixia Yuan* and Yan-Bo Wu*

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Optically active vibrations of extrinsic iron defects in zinc oxide

Alexey N. Kislov* and Anatoly F. Zatsepin

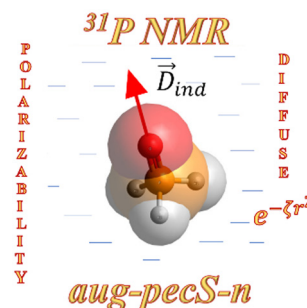


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Going beyond the routine consideration of solvent effects on ^{31}P NMR shielding constants: a meticulous basis set study and new aug-pecS- n ($n = 1$ and 2) basis sets for phosphorus atoms

Yuriy Yu. Rusakov, Yuliya A. Nikurashina and Irina L. Rusakova*



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Macrocyclic *meta*-carborane hexamer. Evaluation of aromatic characteristics as a cluster-based analog to phenyl-bridged macrocyclic structures

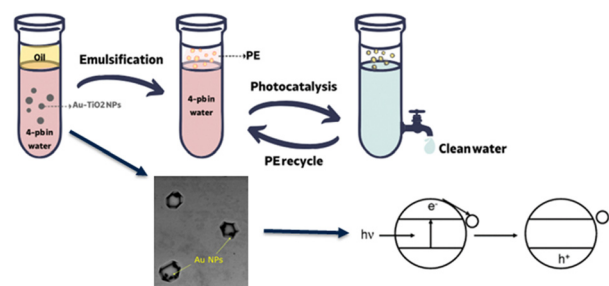
Peter L. Rodriguez-Kessler and Alvaro Muñoz-Castro*



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Dual-functional Au–TiO₂ nanoparticles: enhanced photocatalytic activity and Pickering emulsion stabilization for wastewater treatment

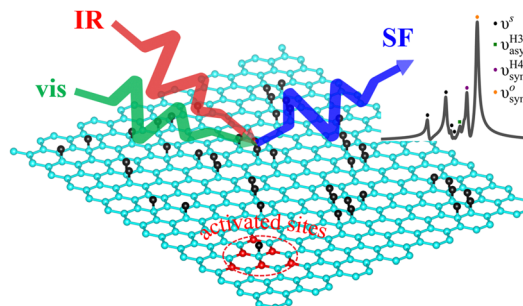
Zygimantas Gričius, Laurine Mroz and Gisle Øye*



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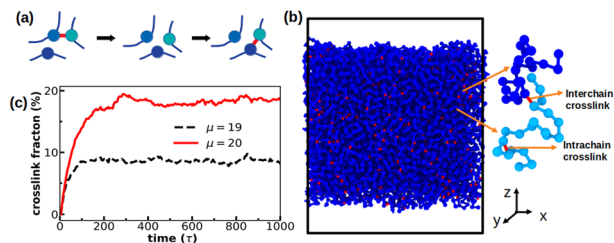
A theoretical study on the formation mechanism and the sum-frequency generation spectra of hydrogenated graphene

Shenghao Cui, Song Zhang, Qing Wang, Fumin Li, Zhitao Shen* and Zhiying Ma*



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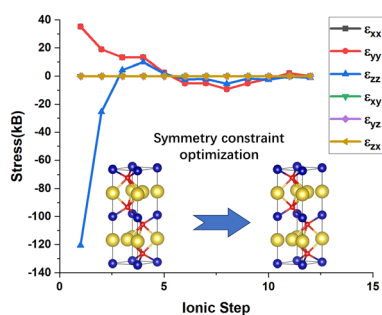
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Rouse mode analysis of chain relaxation in reversibly crosslinked polymer melts

Rahul Karmakar, Srikanth Sastry, Sanat K. Kumar* and Tarak K. Patra*

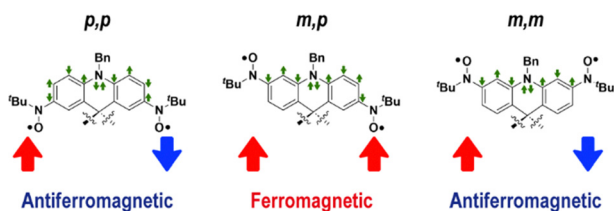
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On-the-fly optimization of the lattice parameters with a symmetry constraint for high-throughput calculation

Shengyi Li, Li Xu,* Cun Wang, Xuechun Wang, Yijie Hou, Peng Sheng, Huitao Bai, Hui Li, Qing Xue and Yumin Qian*

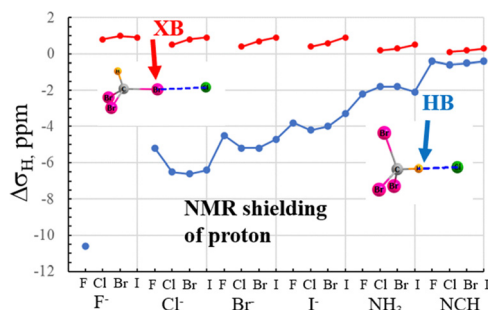
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Radical site-dependent exchange interactions in acridane-based bisnitroxides

Yuta Takenouchi, Takuya Kanetomo* and Masaya Enomoto*

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The competitive strengths of hydrogen and halogen bonding to haloforms and their different spectroscopic markers

Steve Scheiner



CORRECTION

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Correction: Achieving 9% EQE in light-emitting electrochemical cells *via* a TADF-sensitized fluorescence strategy

Zeyang Zhou, Qingda Chang, Rui Chen, Pengfei Jin, Baipeng Yin,* Chuang Zhang* and Jiannian Yao

