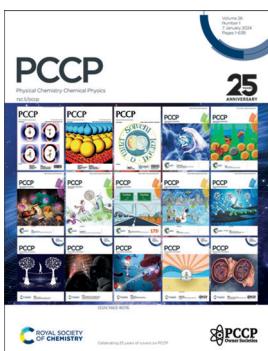


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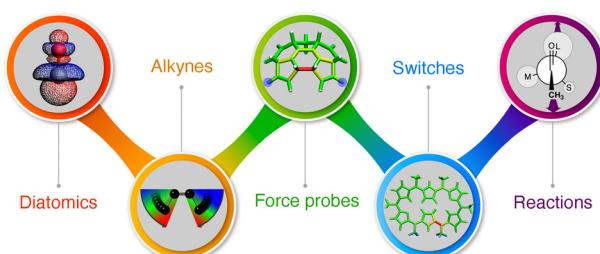
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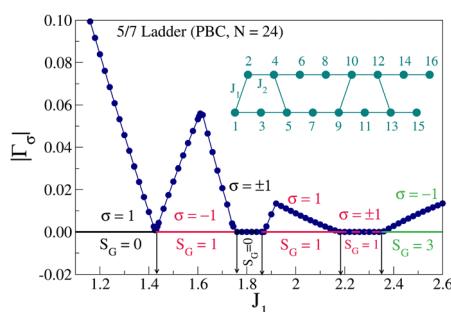
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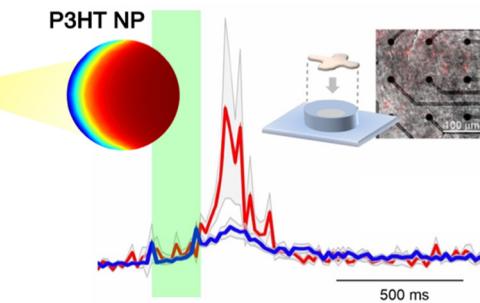
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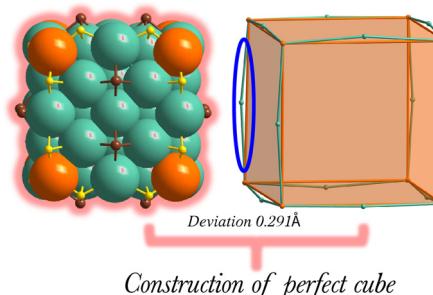
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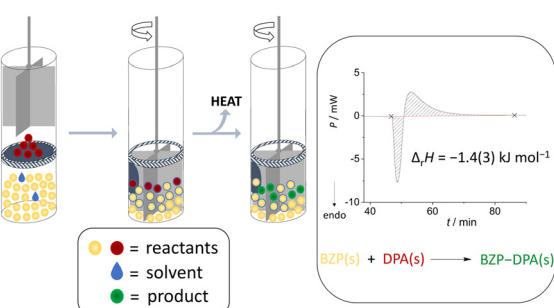


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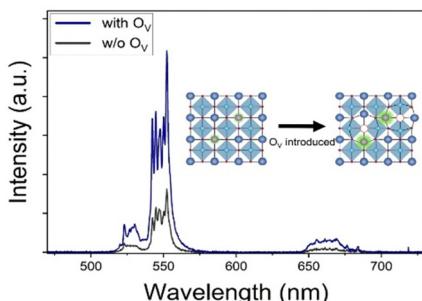
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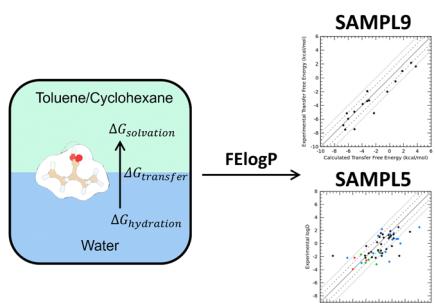
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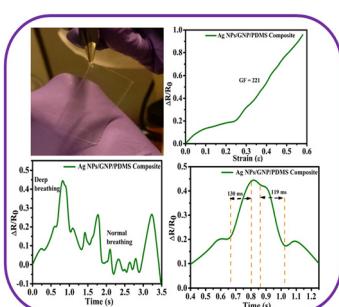
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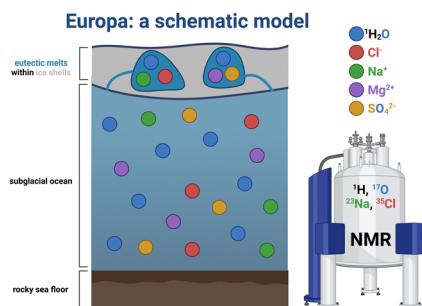
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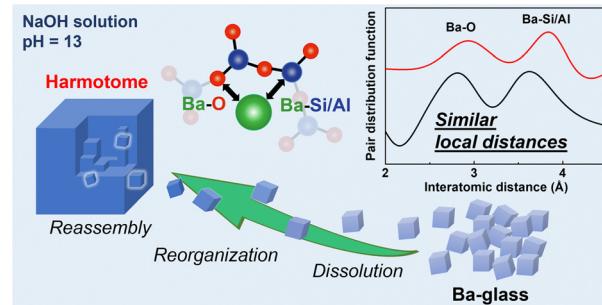


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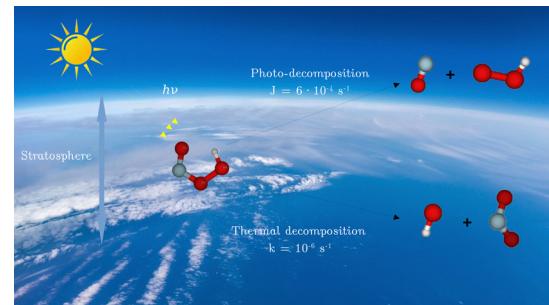
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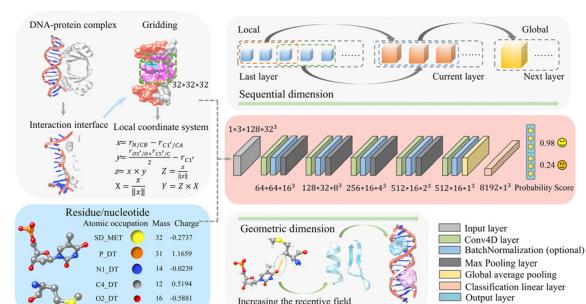
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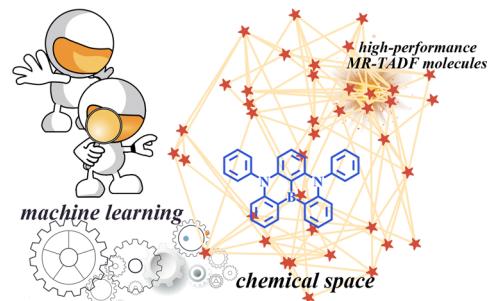
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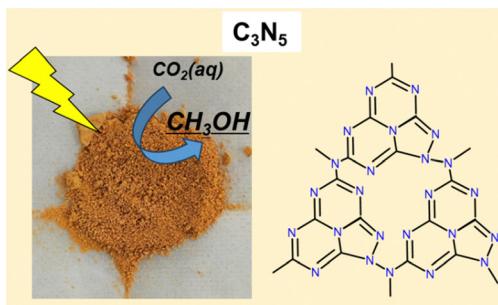
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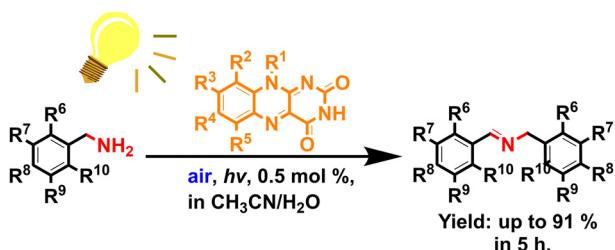
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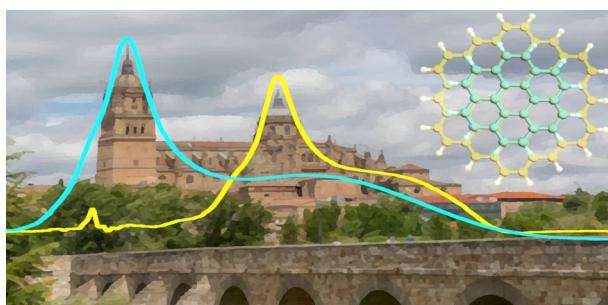
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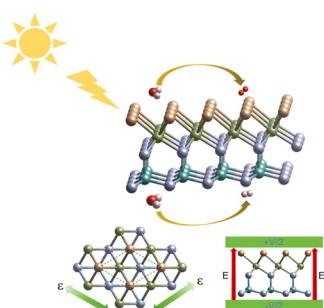
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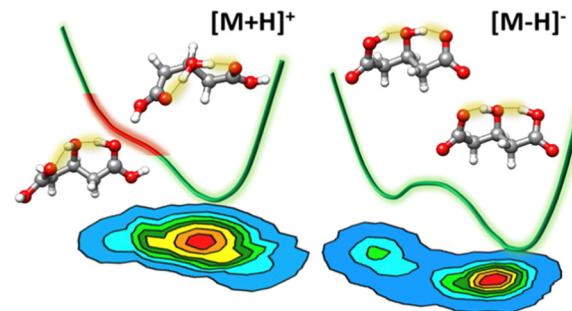


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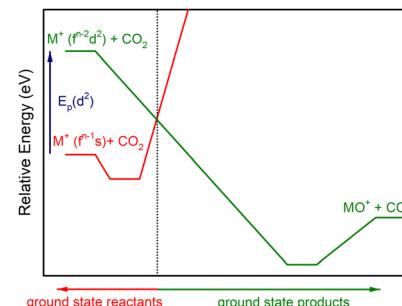
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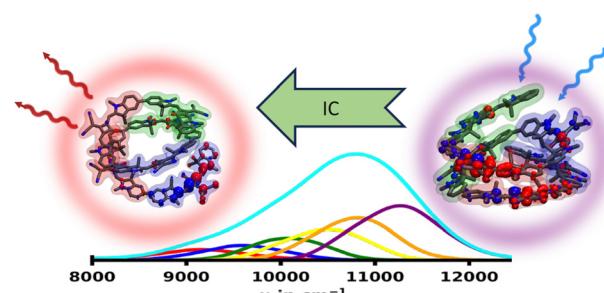
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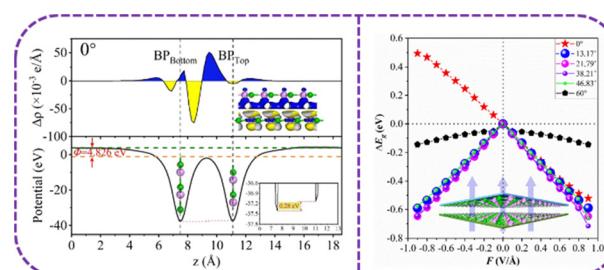
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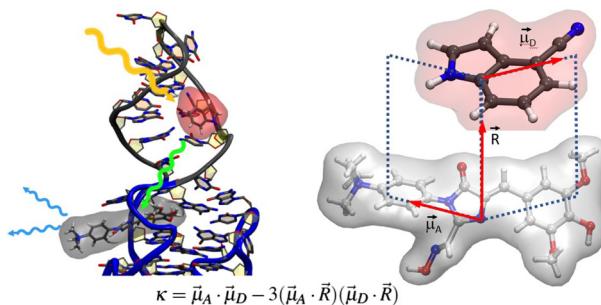
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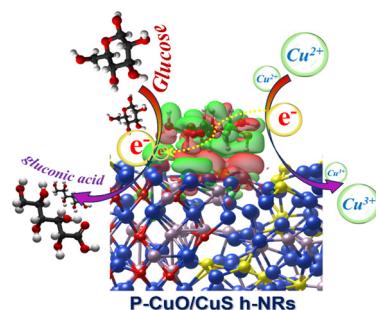
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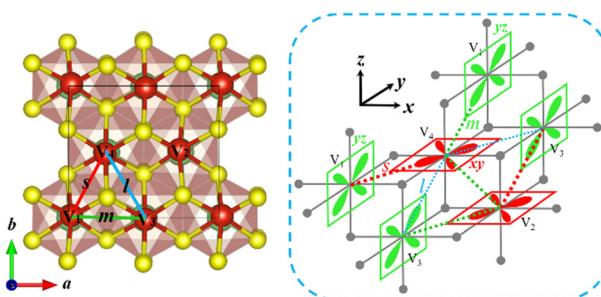
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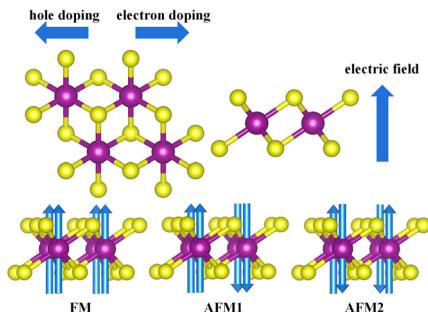
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Structural dimerization and charge-orbital ordering in a ferromagnetic semiconductor LiV₂S₄ monolayer

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Charge doping and electric field tunable ferromagnetism and Curie temperature of the MnS₂ monolayer

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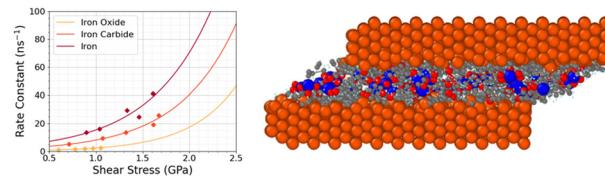


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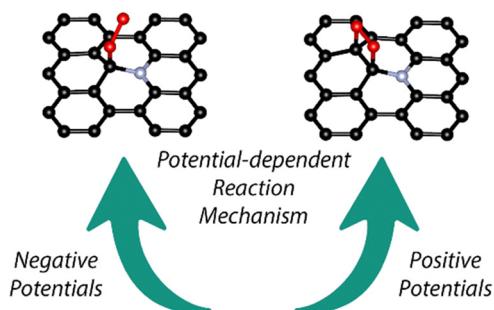
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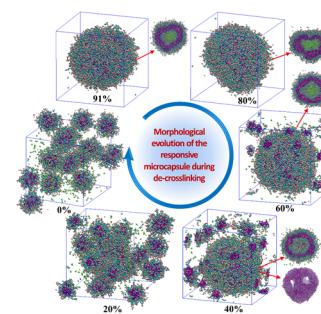
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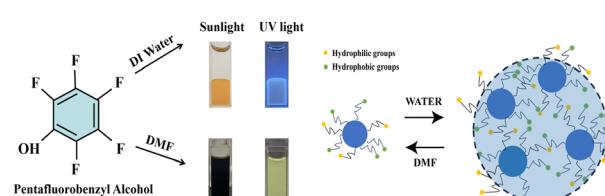
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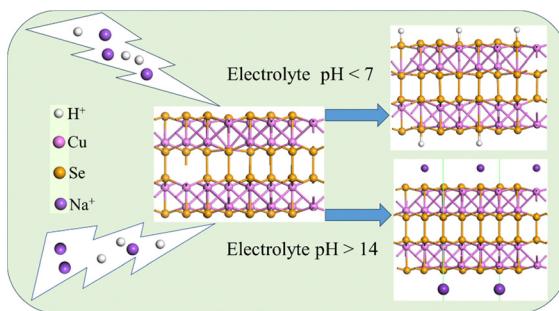
Solvent-controlled synthesis of hydrophilic and hydrophobic carbon dots

Chenhan Zhang, Zhihua Ying,* Yuan Jiang,* Haiyang Wang, Xuebin Zhou, Weipeng Xuan and Peng Zheng



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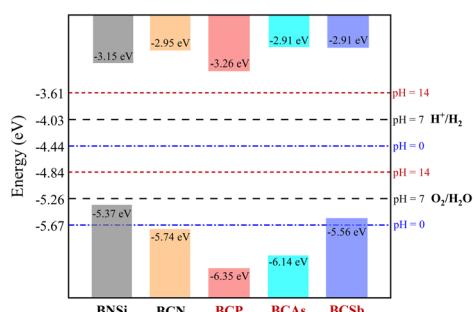
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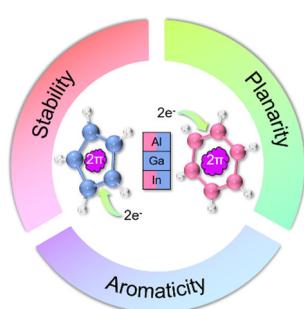
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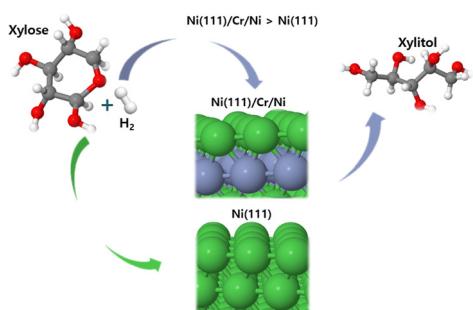
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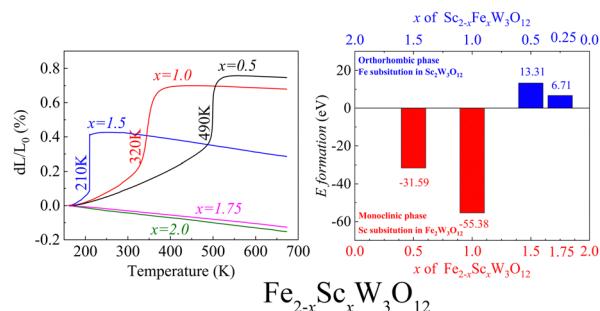


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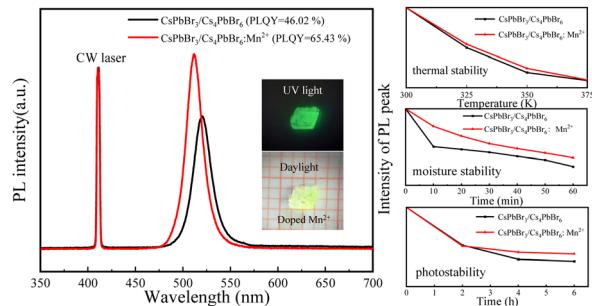
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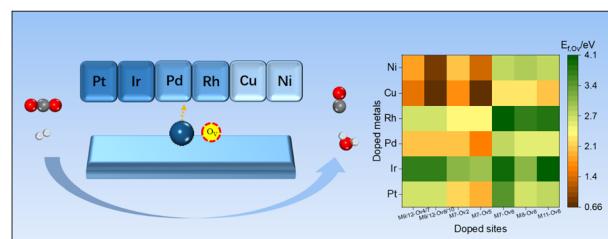
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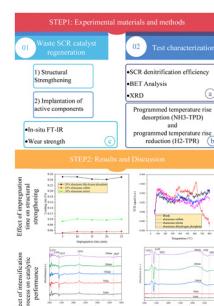
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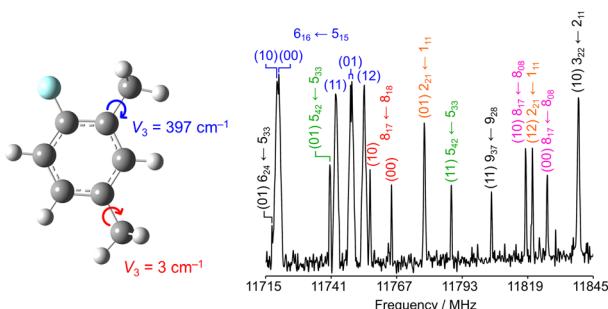
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Dongliang Ji, Dongxue Jiang, Yang Li, Huan Zhang, Haiyun Zhou, Zhaoqin Huang* and Jianzhong Zhu*



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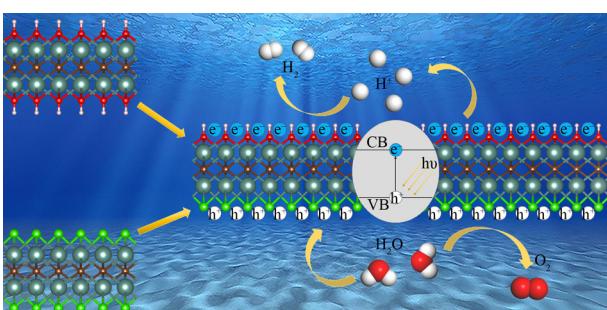
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Approaching the free rotor limit: extremely low methyl torsional barrier observed in the microwave spectrum of 2,4-dimethylfluorobenzene

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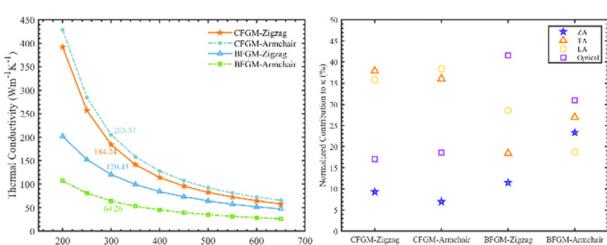
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Sheng-Yi Zhang, Ni-Ping Shi, Chuan-Kui Wang* and Guang-Ping Zhang*

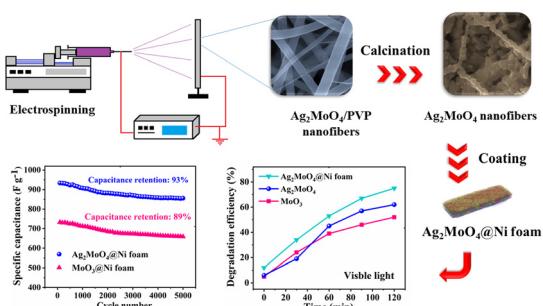
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First-principles prediction of the thermal conductivity of two configurations of difluorinated graphene monolayer

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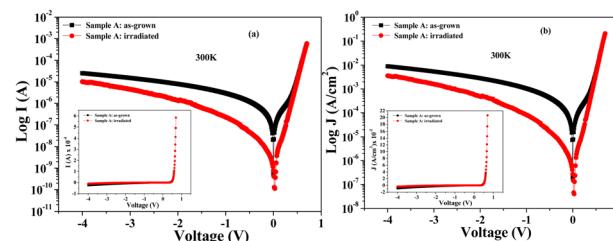


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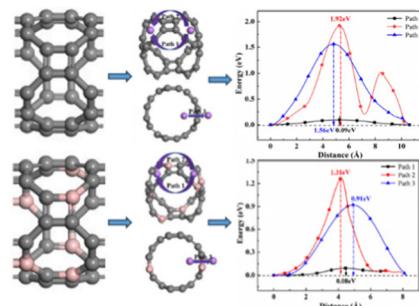
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Exploring the structural stability and electrochemical performance of B doped T-graphene nanotubes from first-principles calculations

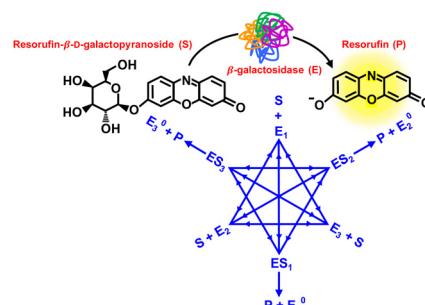
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A minimal kinetic model for the interpretation of complex catalysis in single enzyme molecules

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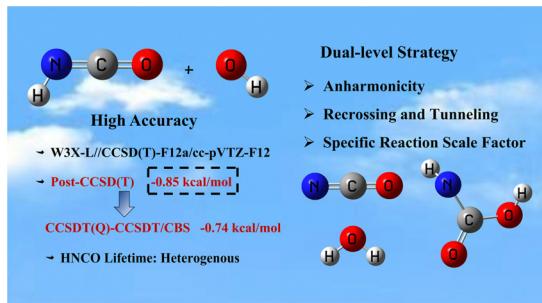
Halogen bond catalysis of the [4+2] cycloaddition reaction of 2-alkenylindoles: catalytic modes and stereoselectivity

Ying Li, Chang Zhao, Huaiyu Zhang* and Yanli Zeng*



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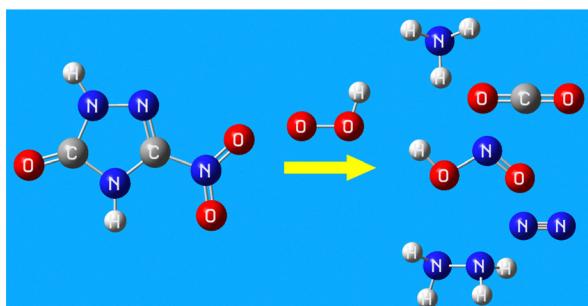
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Quantitative kinetics of the atmospheric reaction between isocyanic acid and hydroxyl radicals: post-CCSD(T) contribution, anharmonicity, recrossing effects, torsional anharmonicity, and tunneling

Dai-Dan Deng and Bo Long*

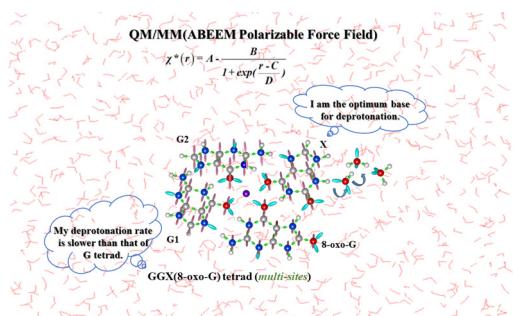
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Liudmyla K. Sviatenko, Leonid Gorb and Jerzy Leszczynski*

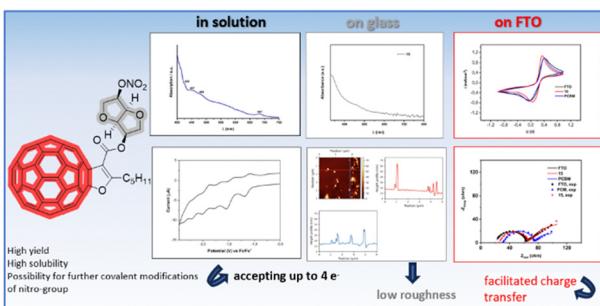
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Development of a QM/MM(ABEEM) method for the deprotonation of neutral and cation radicals in the G-tetrad and GGX(8-oxo-G) tetrad

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Exploring fullerene derivatives for optoelectronic applications: synthesis and characterization study

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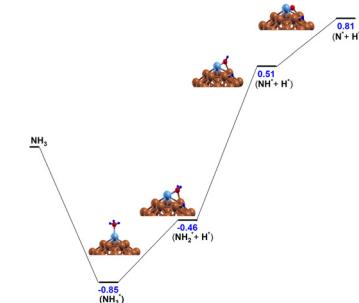


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Adsorption and dehydrogenation of ammonia on Ru₅₅, Cu₅₅ and Ru@Cu₅₄ nanoclusters: role of single atom alloy catalyst

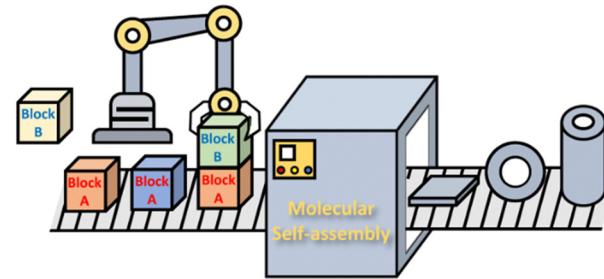
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Self-assembly morphology transition mechanism of similar amphiphilic molecules

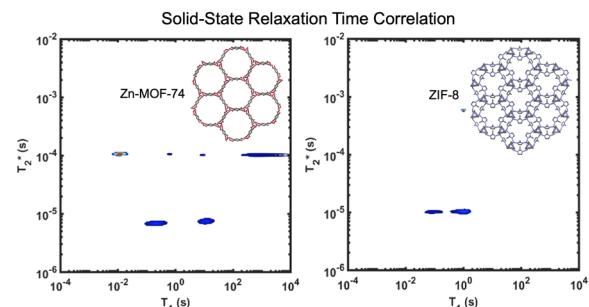
Junben Weng, Haojiang Yao, Junfeng Wang* and Guohui Li*



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In situ monitoring of mechanochemical MOF formation by NMR relaxation time correlation

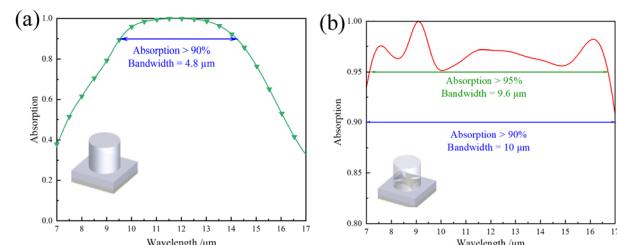
Madeleine E. Leger, Jiangfeng Guo, Bryce MacMillan, Hatem M. Titi, Tomislav Friščić, Bruce Balcom* and Barry A. Blight*



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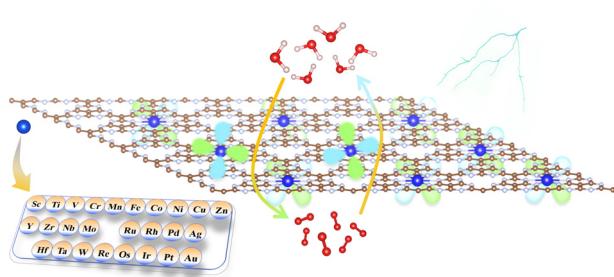
Design of metamaterial perfect absorbers in the long-wave infrared region

Yang Wang, Xiu Li, Shenbing Wu, Changjun Hu and Yuanyuan Liu*



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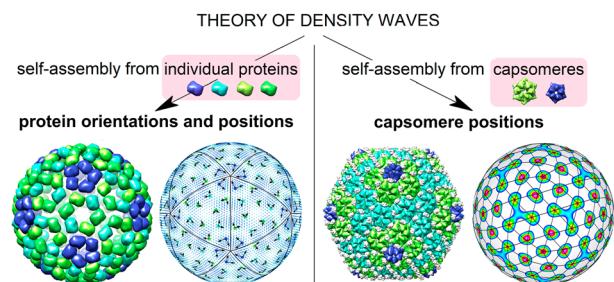
558



The regulatory function of the d-orbital structure in TM@g-t-C₄N₃ for bifunctional catalysis of the oxygen evolution/reduction reaction

Zhenduo Wang, Meichen Wu, Yuhong Huang, Jianmin Zhang* and Xiumei Wei*

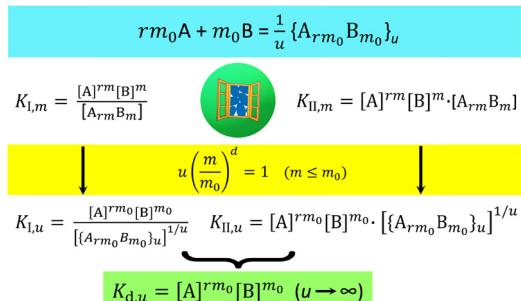
569



Theory of density waves and organization of proteins in icosahedral virus capsids

Olga V. Konevtsova, Dmitrii V. Chalin and Sergei B. Rochal*

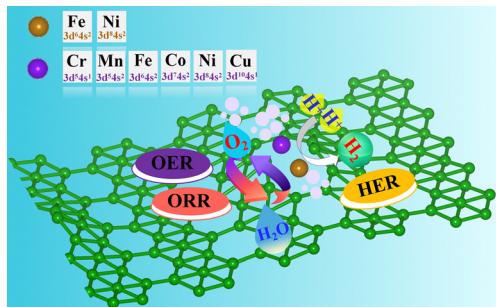
581



Pseudo-equilibrium equations for calcium phosphate precipitation with multi-unit particles

Tian-Lan Zhang

594



Bifunctional diatomic site catalysts supported by β_{12} -borophene for efficient oxygen evolution and reduction reactions

Jia Liu, Minjing Zhang, Si-Dian Li* and Yuewen Mu*

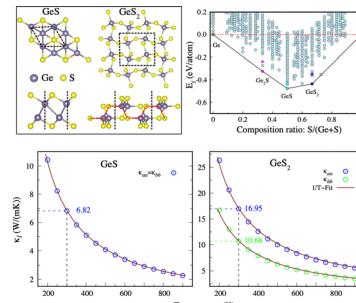


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602

Prediction of novel ground-state structures and analysis of phonon transport in two-dimensional Ge_xS_y compounds

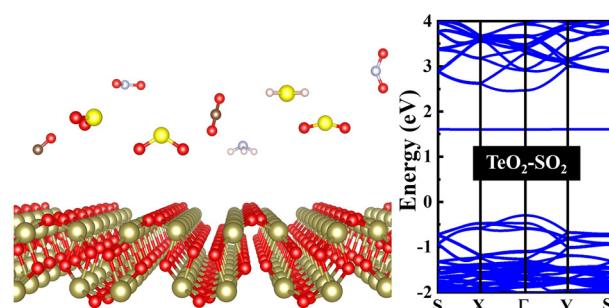
Asad Ali and Young-Han Shin*



612

Adsorption and sensing performance of air pollutants on a $\beta\text{-TeO}_2$ monolayer: a first-principles study

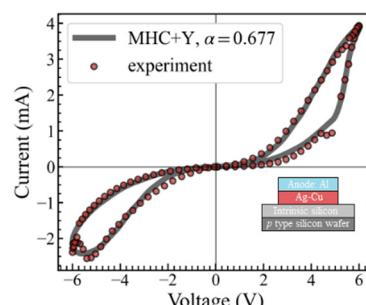
Ying Wang, Shiying Guo,* Xiaoyong Xu, Jing Pan, Jingguo Hu and Shengli Zhang*



621

Fractional Marcus–Hush–Chidsey–Yakopcic current–voltage model for redox-based resistive memory devices

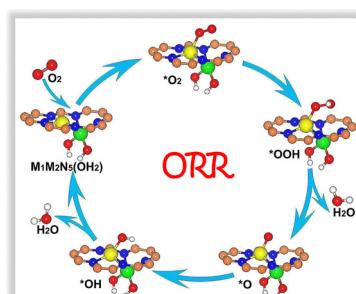
G. V. Paradezhenko,* D. V. Prodan, A. A. Pervishko, D. Yudin and A. Allagui



628

Boosting the oxygen reduction reaction activity of dual-atom catalysts on N-doped graphene by regulating the N coordination environment

Lei Li,* Xiaoxia Wu, Qiuying Du, Narsu Bai and Yuhua Wen*



CORRECTION

635

Correction: Structural, electronic, optical, elastic, thermodynamic and thermal transport properties of $\text{Cs}_2\text{AgInCl}_6$ and $\text{Cs}_2\text{AgSbCl}_6$ double perovskite semiconductors using a first-principles study

Keqing Zhang, Lijun Zhang, S. K. S. Saravana Karthikeyan, Chang Yi Kong, Fuchun Zhang, Xiang Guo,* Nam Nguyen Dang, Sankar Ganesh Ramaraj* and Xinghui Liu*

