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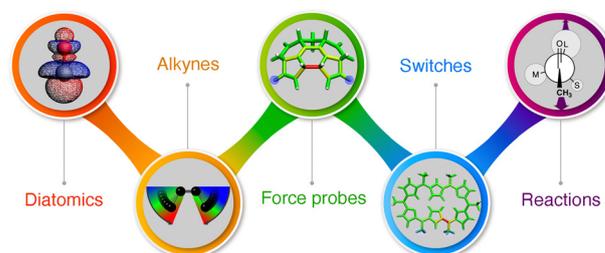
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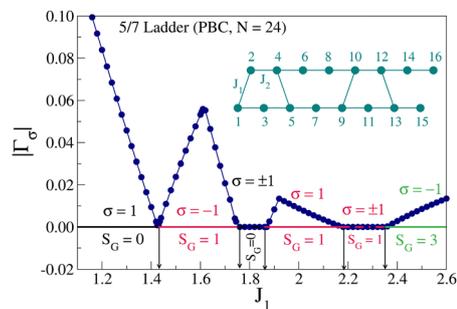
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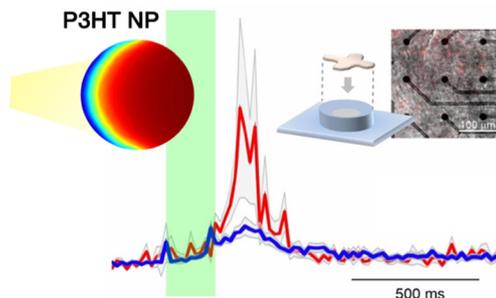


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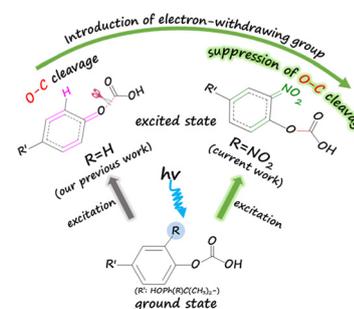
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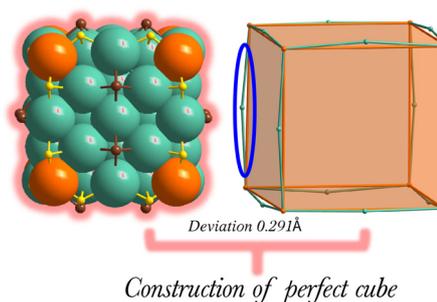
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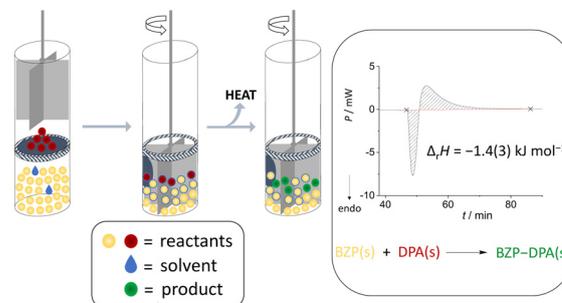


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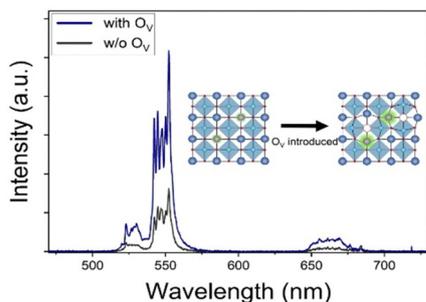
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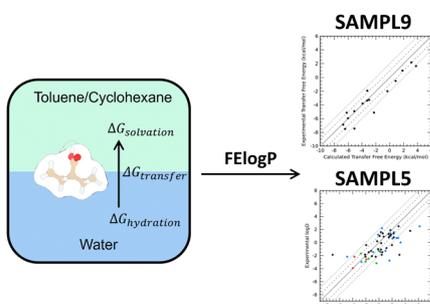
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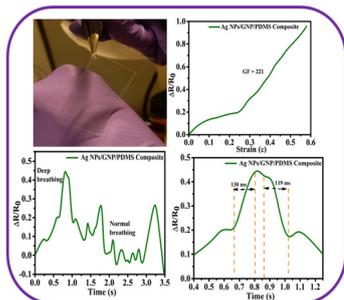
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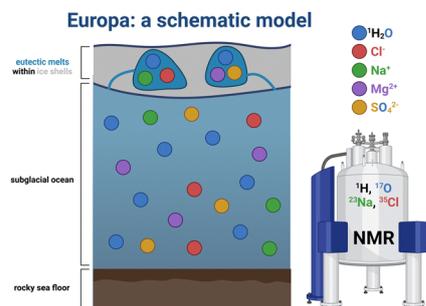
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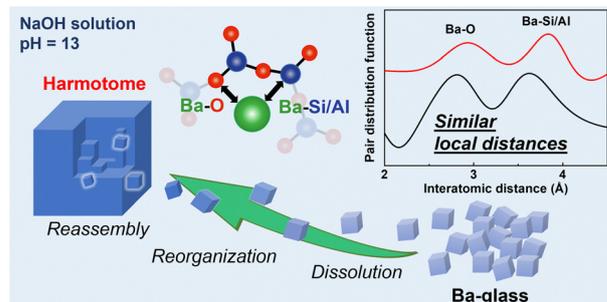
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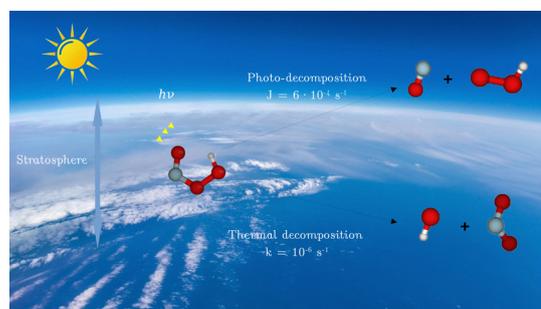
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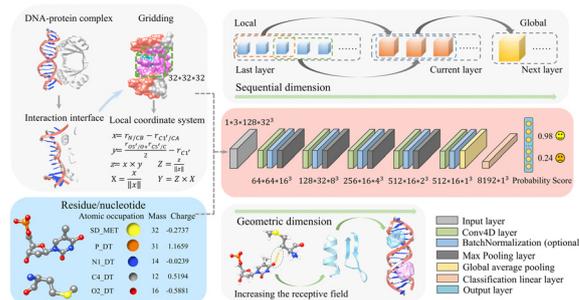
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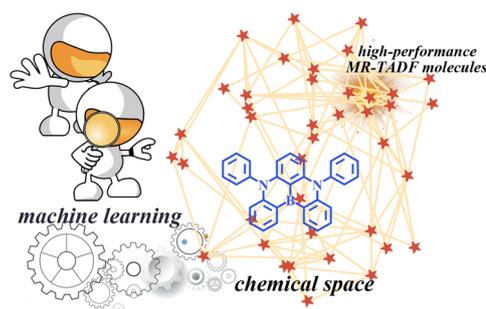
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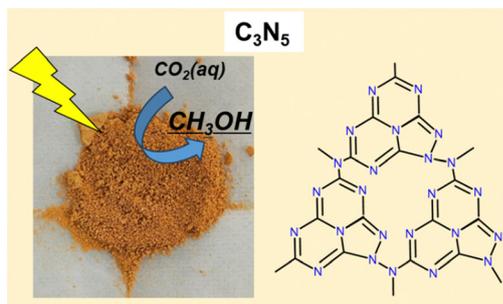
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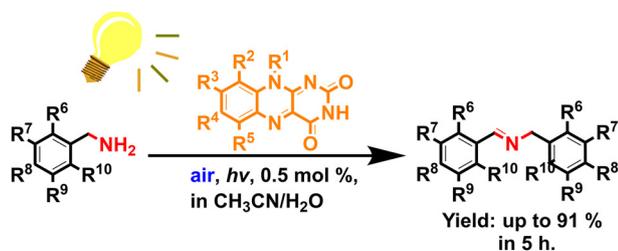
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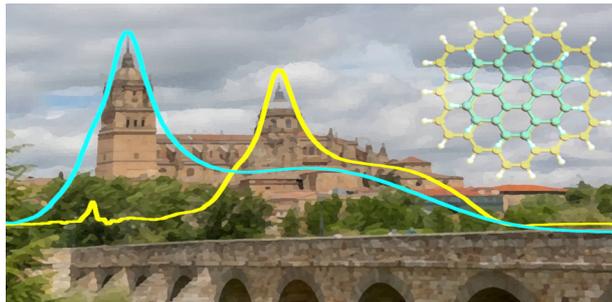
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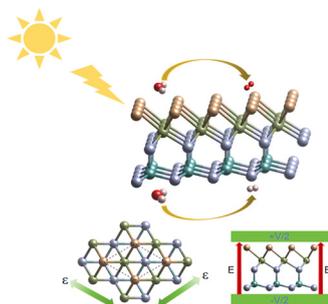
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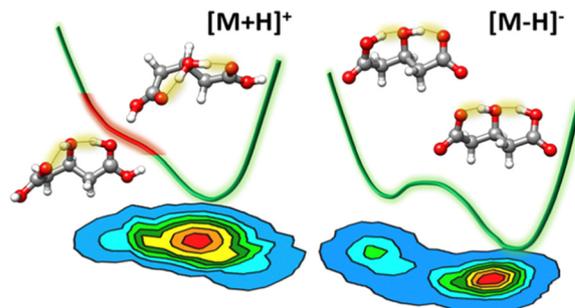


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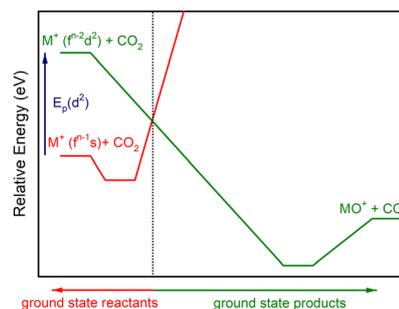
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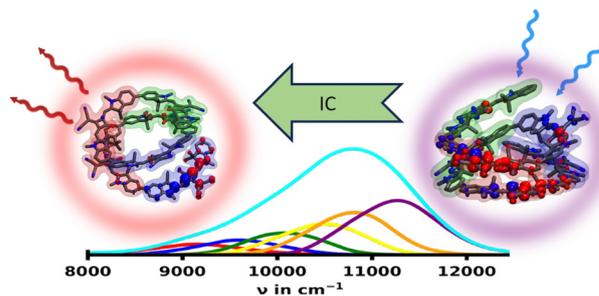
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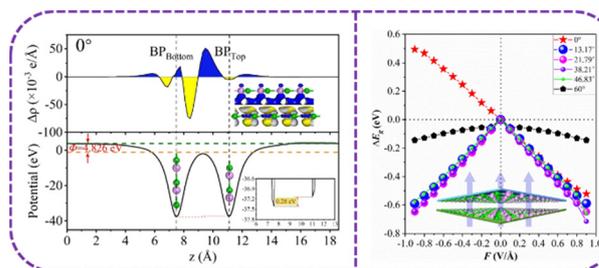
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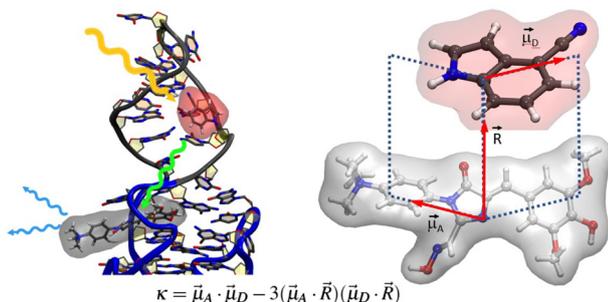
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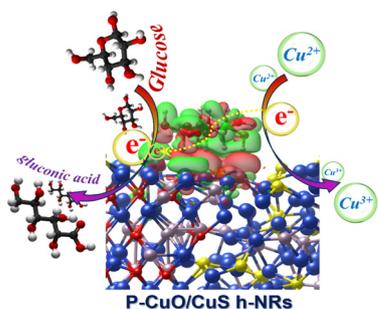
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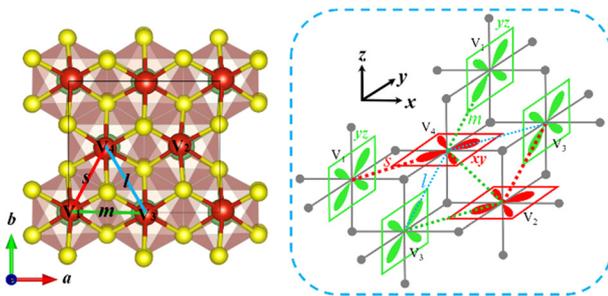
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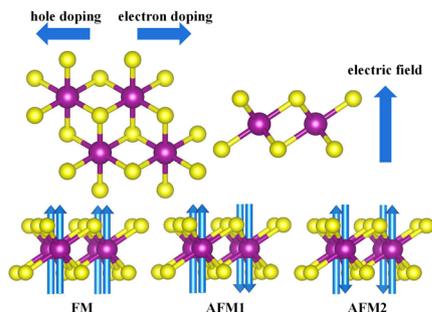
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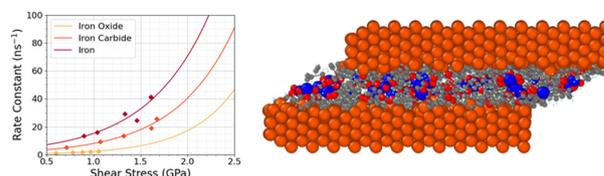
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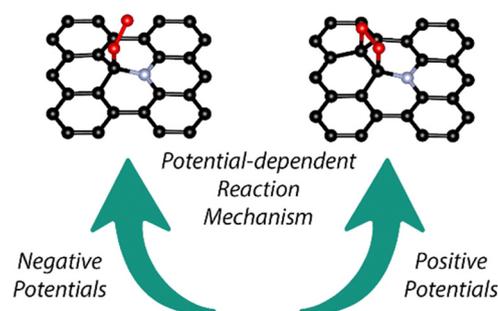
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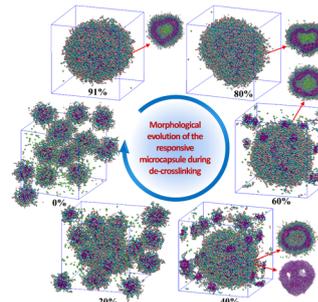
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A dissipative particle dynamics simulation of controlled loading and responsive release of theranostic agents from reversible crosslinked triblock copolymer vesicles

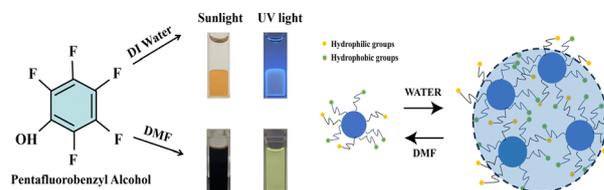
Zhikun Wang, Fengting Li, Li Wang, Yueqi Liu, Miantuo Li, Nannan Cui, Chunling Li, Shuangqing Sun* and Songqing Hu*



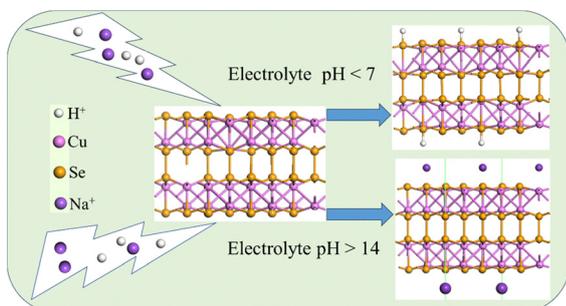
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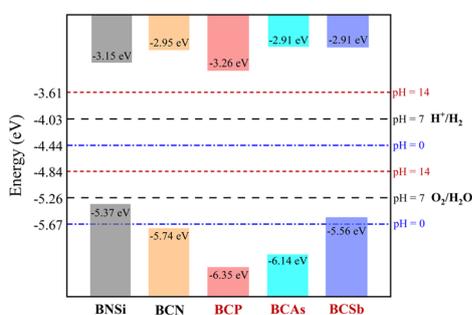
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Theoretical insights into surface-phase transition and ion competition during alkali ion intercalation on the Cu_4Se_4 nanosheet

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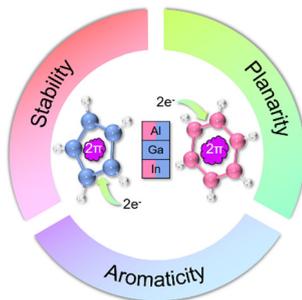
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Two-dimensional ternary pentagonal BCX (X = P, As, and Sb): promising photocatalyst semiconductors for water splitting with strong piezoelectricity

Luqi Liu, Xuxin Kang, Shan Gao* and Xiangmei Duan*

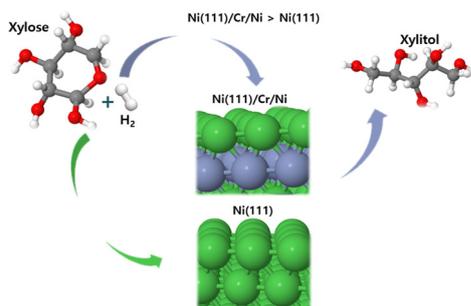
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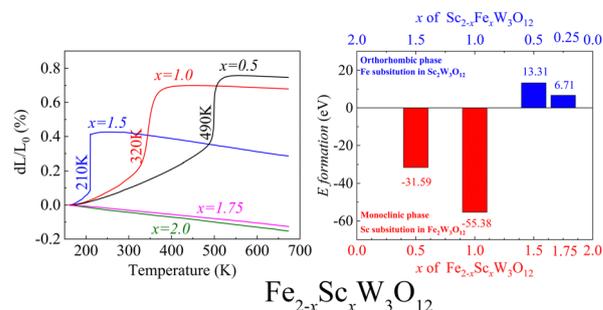


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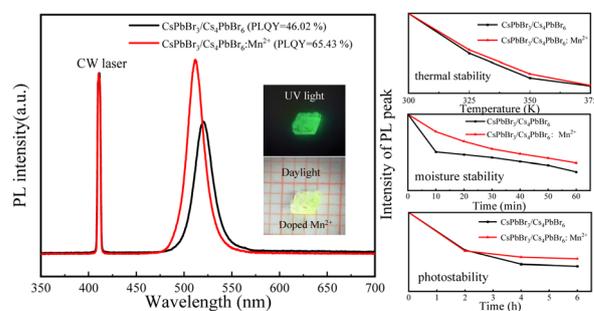
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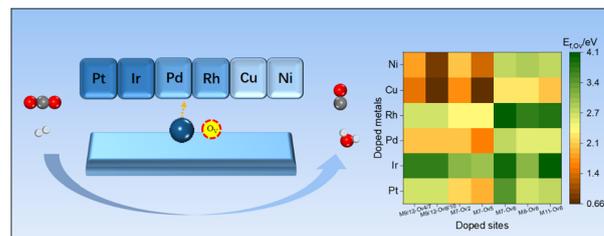
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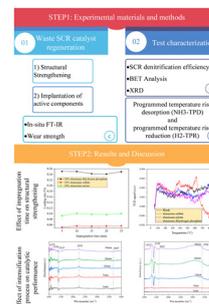
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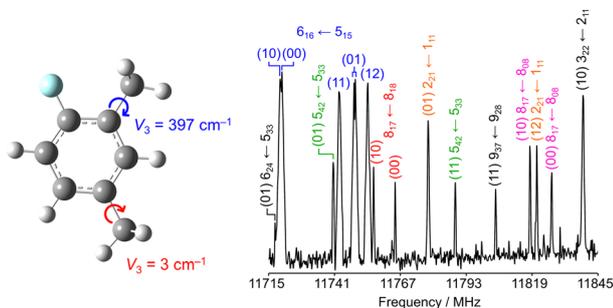
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Research on structural strengthening technology for regenerative denitration catalysts

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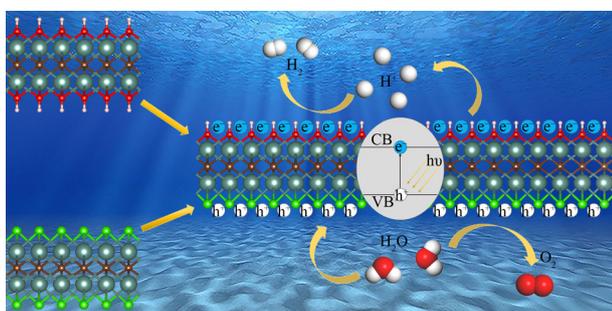
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Approaching the free rotor limit: extremely low methyl torsional barrier observed in the microwave spectrum of 2,4-dimethylfluorobenzene

Safa Khemissi,* Martin Schwell, Isabelle Kleiner and Ha Vinh Lam Nguyen*

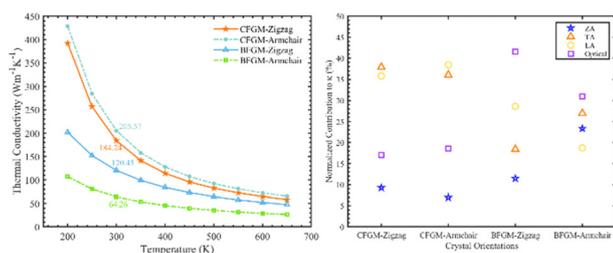
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First-principles studies on the electronic and photocatalytic water splitting properties of surface functionalized Y₂C-based MXenes

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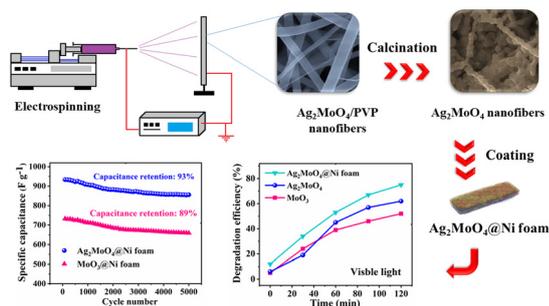
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Novel electrospun bead-like Ag₂MoO₄ nanofibers coated on Ni foam for visible light-driven heterogeneous photocatalysis and high-performance supercapacitor electrodes

Amirreza Safartoobi, Jamal Mazloom* and Farhad Esmaili Ghodsi

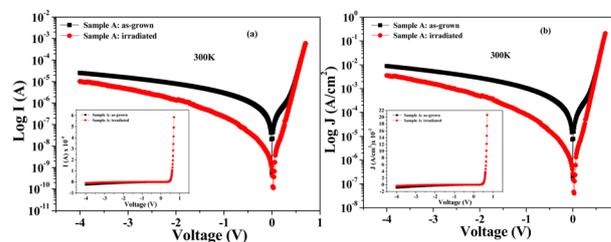


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Effects of gamma radiation on the electrical properties of InAs/InGaAs quantum dot-based laser structures grown on GaAs and Si substrates by molecular beam epitaxy

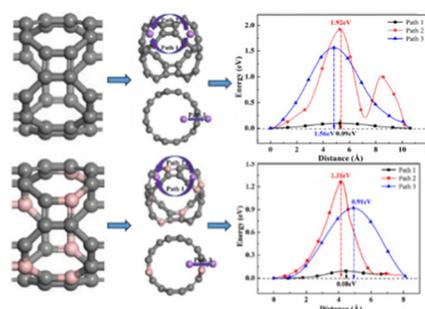
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Exploring the structural stability and electrochemical performance of B doped T-graphene nanotubes from first-principles calculations

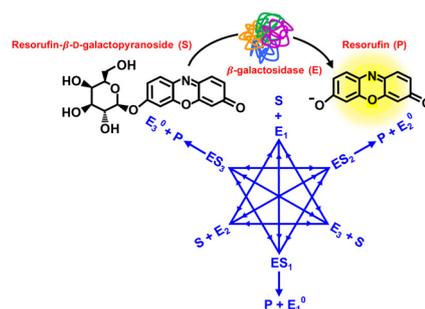
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A minimal kinetic model for the interpretation of complex catalysis in single enzyme molecules

Prasanta Kundu, Soma Saha* and Gautam Gangopadhyay



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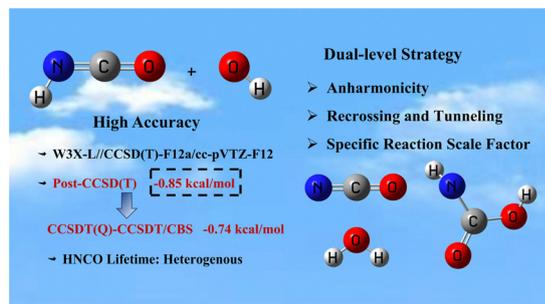
Halogen bond catalysis of the [4+2] cycloaddition reaction of 2-alkenylindoles: catalytic modes and stereoselectivity

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



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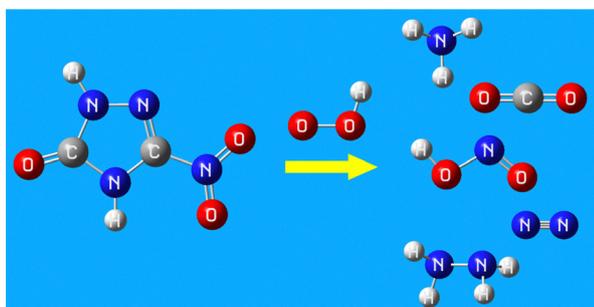
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Quantitative kinetics of the atmospheric reaction between isocyanic acid and hydroxyl radicals: post-CCSD(T) contribution, anharmonicity, recrossing effects, torsional anharmonicity, and tunneling

Dai-Dan Deng and Bo Long*

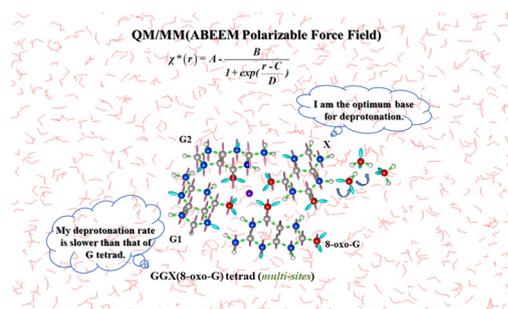
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Degradation of NTO induced by superoxide and hydroperoxyl radicals: a comprehensive DFT study

Liudmyla K. Sviatenko, Leonid Gorb and Jerzy Leszczynski*

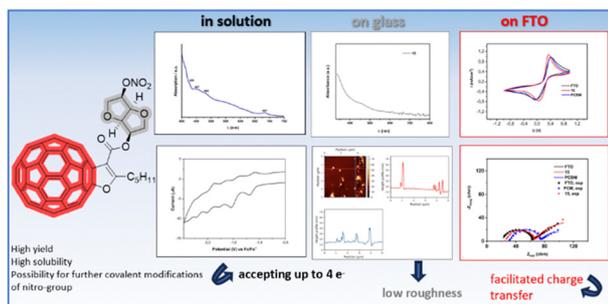
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Development of a QM/MM(ABEEM) method for the deprotonation of neutral and cation radicals in the G-tetrad and GGX(8-oxo-G) tetrad

Yue Wang, Linlin Liu, Yue Gao, Jiayue Zhao, Cui Liu,* Lidong Gong* and Zhongzhi Yang

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Exploring fullerene derivatives for optoelectronic applications: synthesis and characterization study

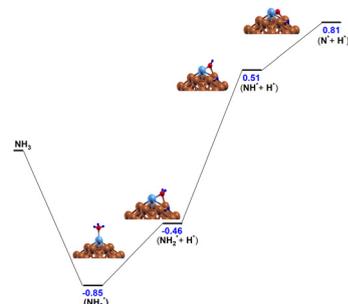
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Adsorption and dehydrogenation of ammonia on Ru_{55} , Cu_{55} and Ru@Cu_{54} nanoclusters: role of single atom alloy catalyst

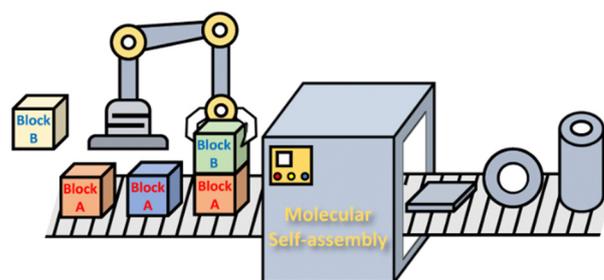
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Self-assembly morphology transition mechanism of similar amphiphilic molecules

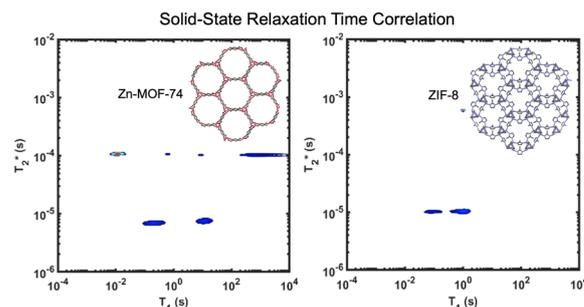
Junben Weng, Haojiang Yao, Junfeng Wang* and Guohui Li*



543

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

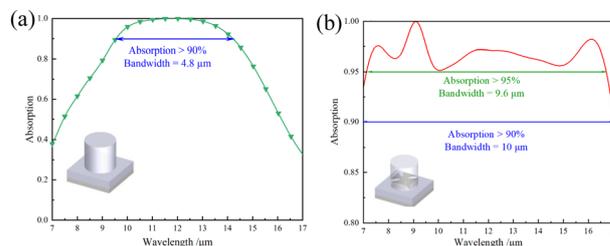
Madeleine E. Leger, Jiangfeng Guo, Bryce MacMillan, Hatem M. Titi, Tomislav Friščić, Bruce Balcom* and Barry A. Blight*



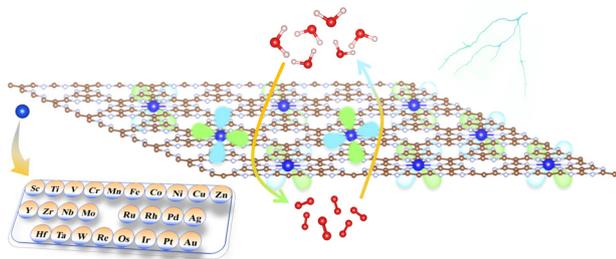
551

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

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



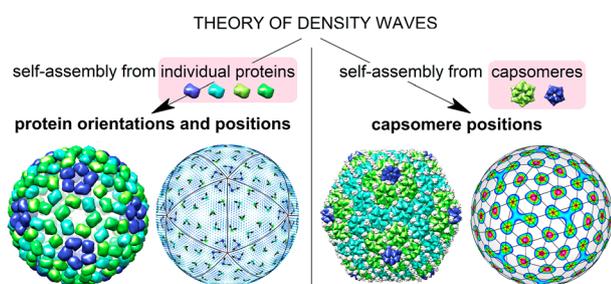
558



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

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

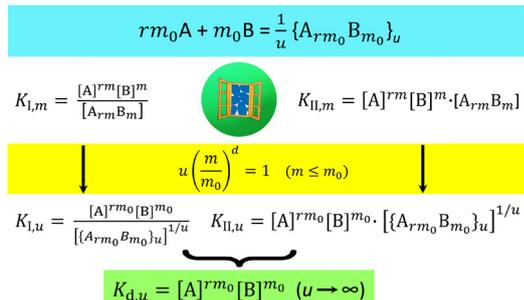
569



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

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

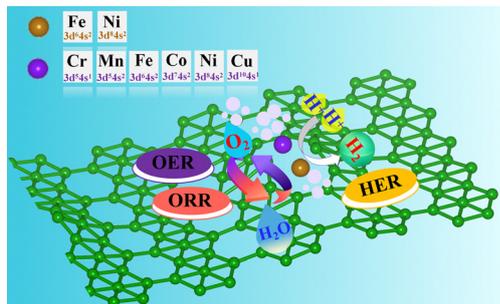
581



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

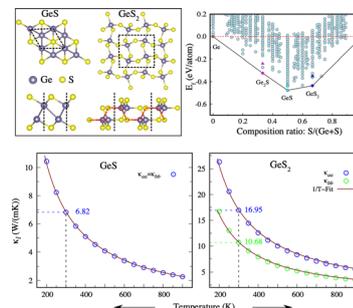
Jia Liu, Minjing Zhang, Si-Dian Li* and Yuewen Mu*



602

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

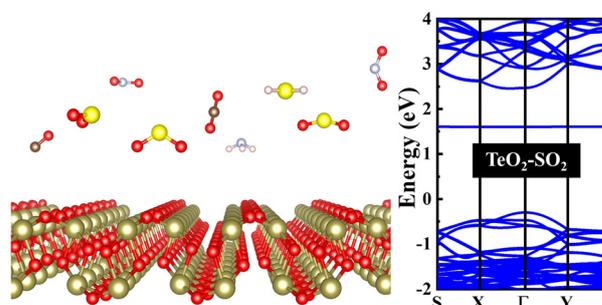
Asad Ali and Young-Han Shin*



612

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

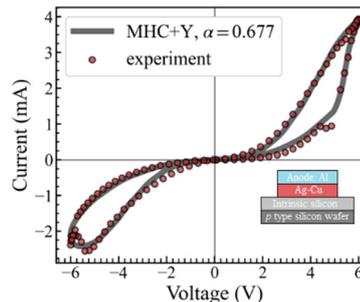
Ying Wang, Shiyong Guo,* Xiaoyong Xu, Jing Pan, Jingguo Hu and Shengli Zhang*



621

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

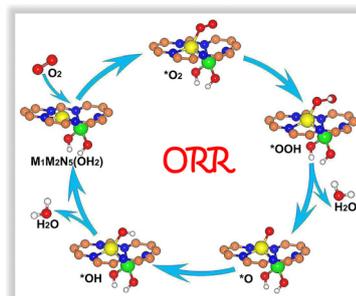
G. V. Paradezhenko,* D. V. Prodan, A. A. Pervishko, D. Yudin and A. Allagui



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*

