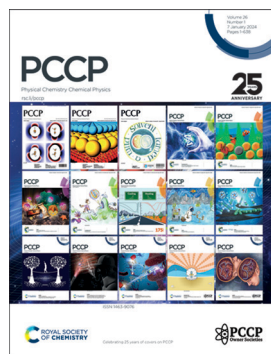


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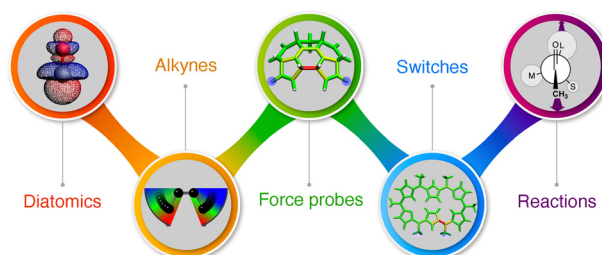
**Inside cover**  
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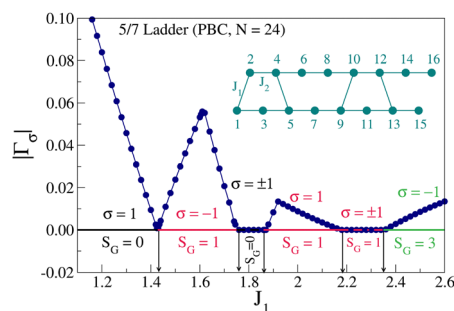
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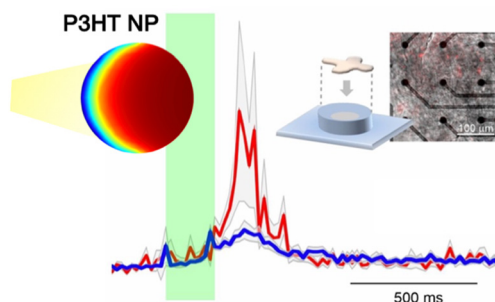


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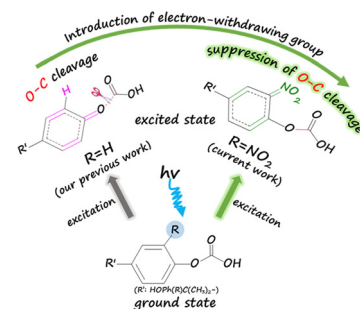
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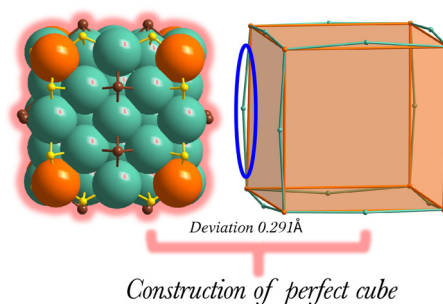
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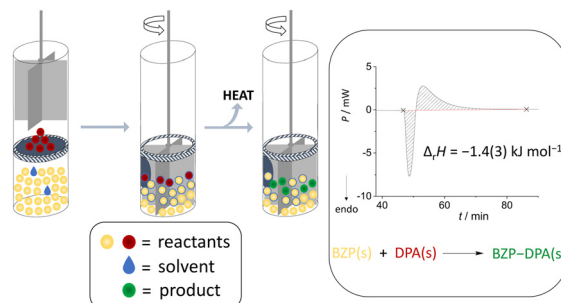


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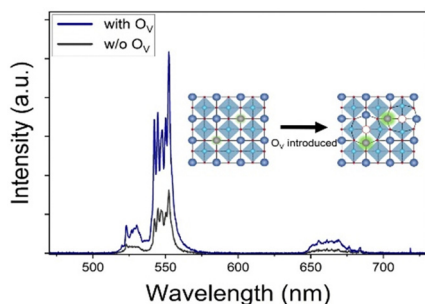
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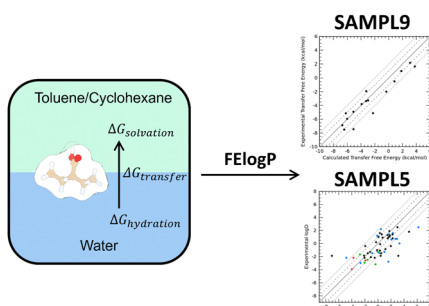
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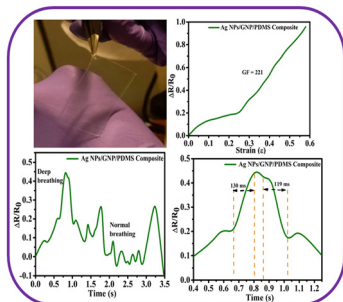
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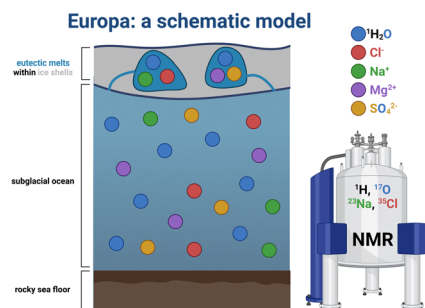
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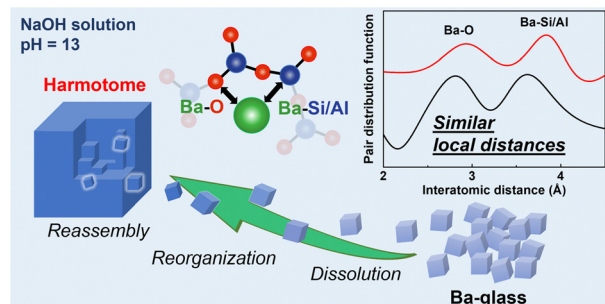


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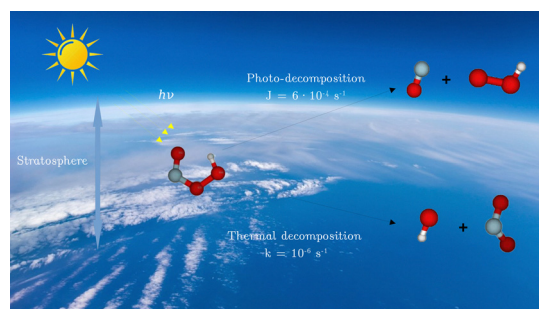
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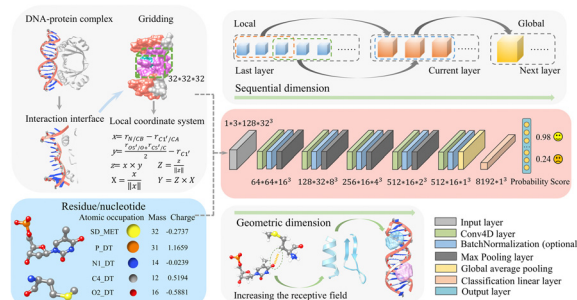
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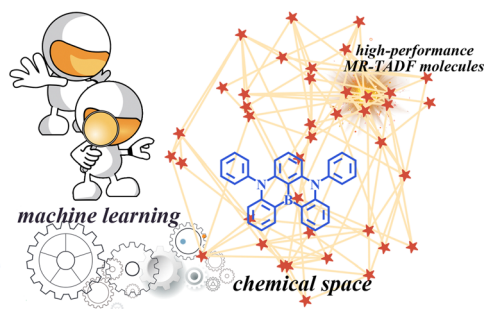
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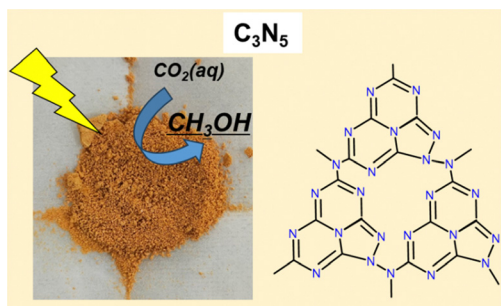
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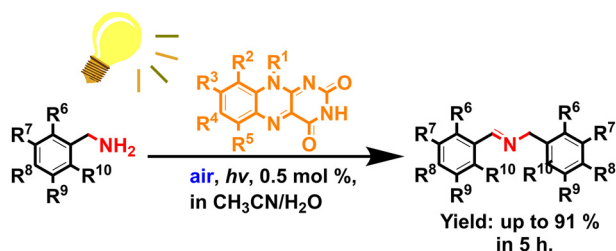
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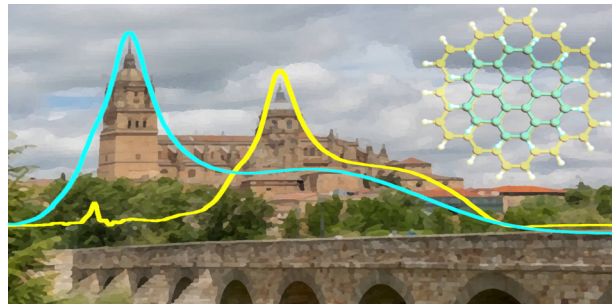
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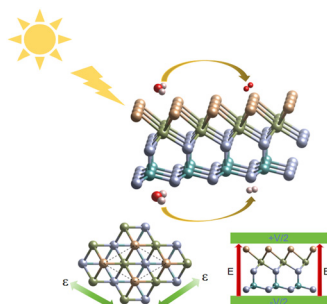
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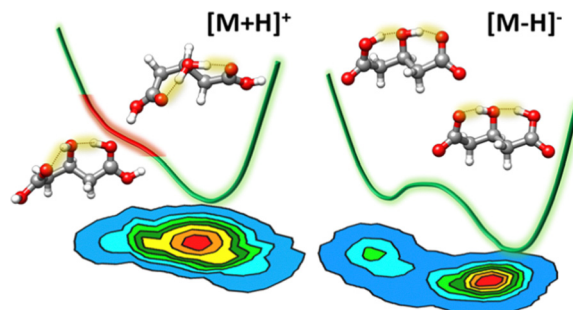


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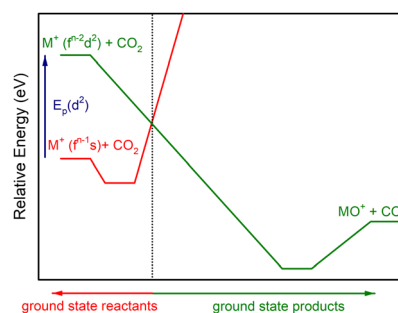
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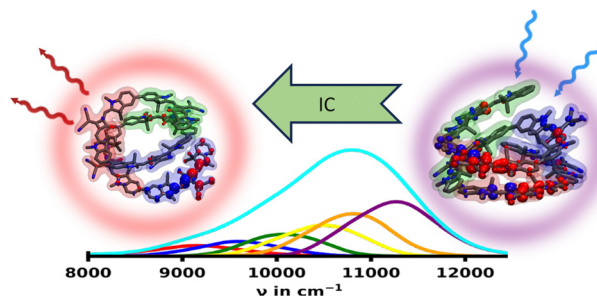
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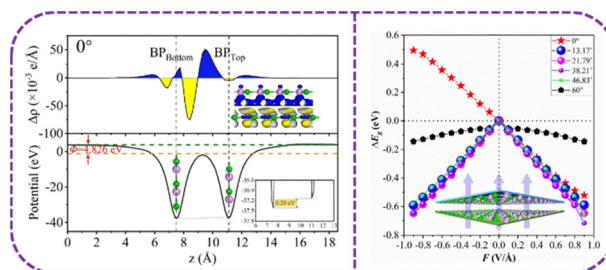
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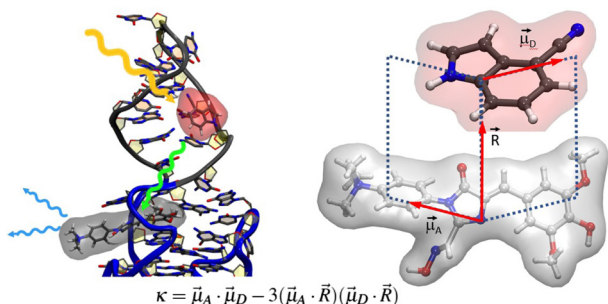
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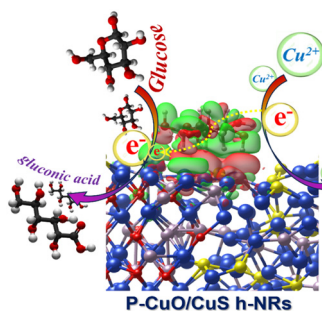
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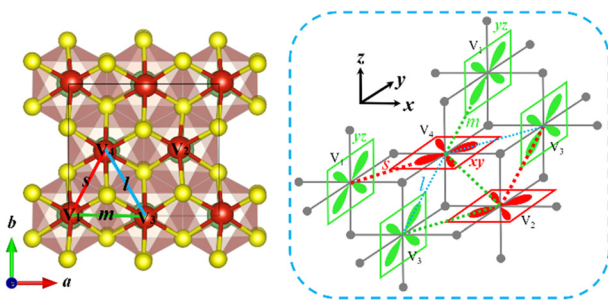
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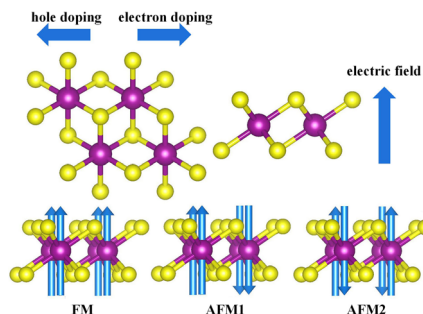
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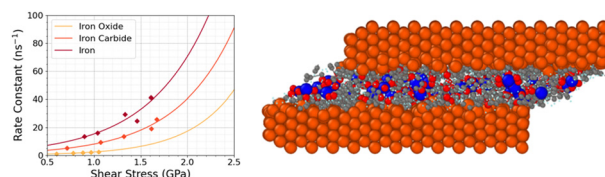


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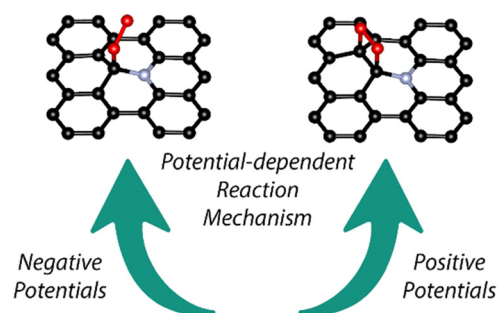
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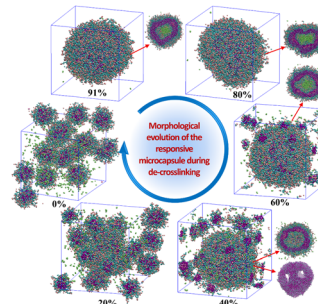
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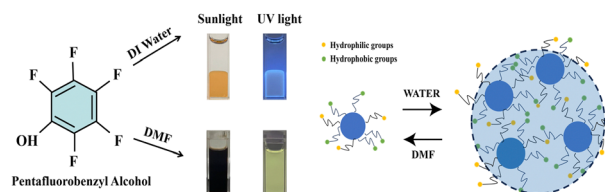
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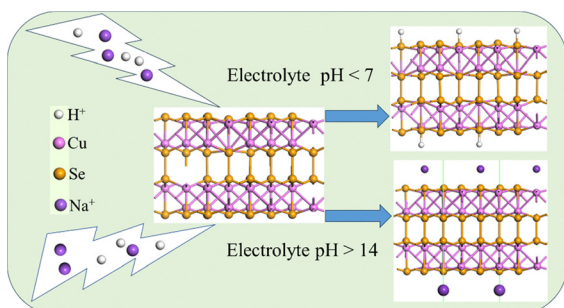
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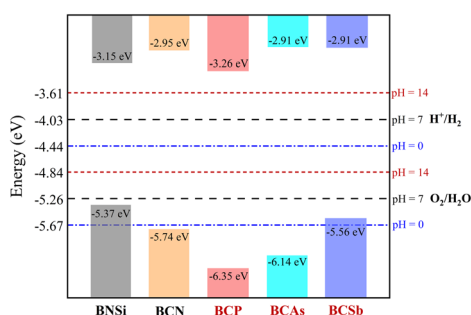
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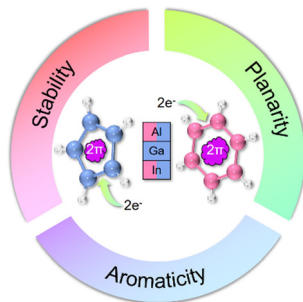
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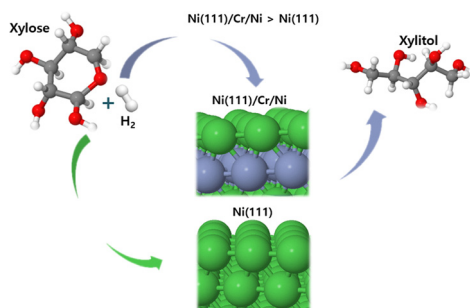
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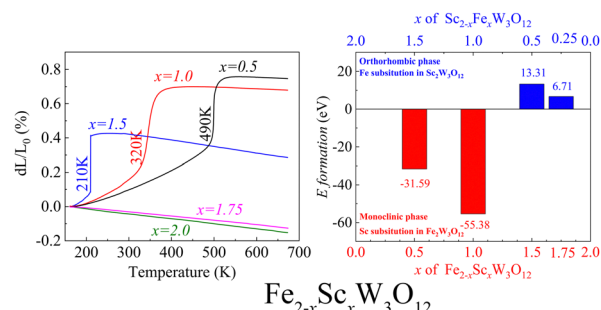


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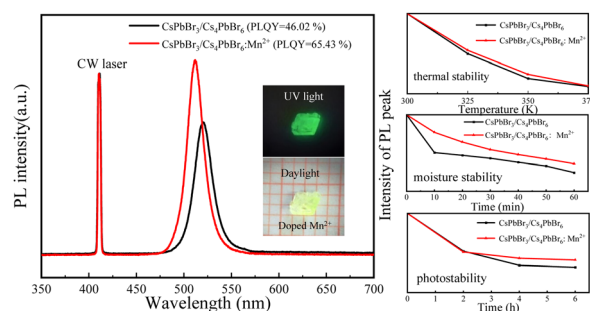
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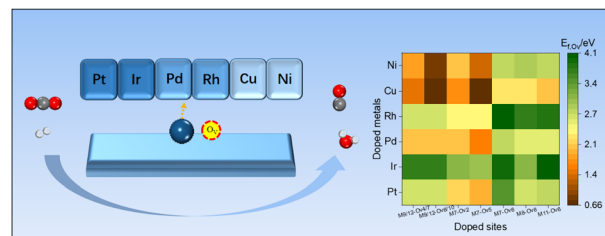
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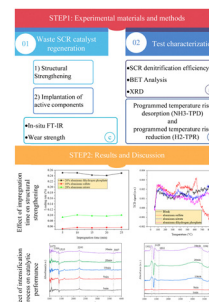
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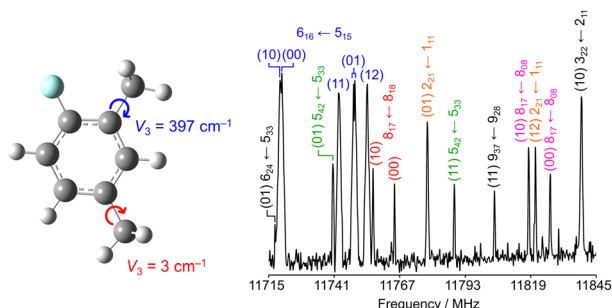
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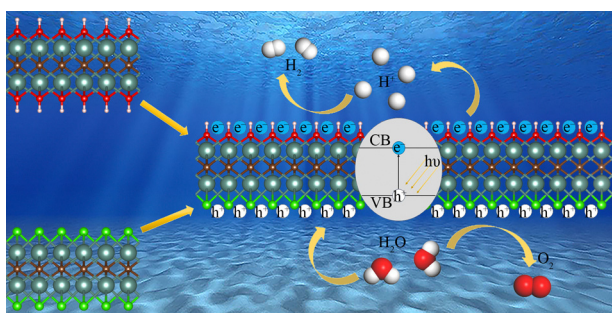
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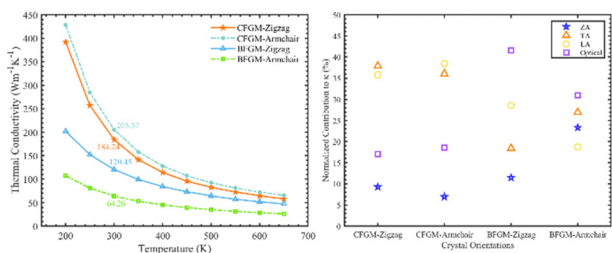
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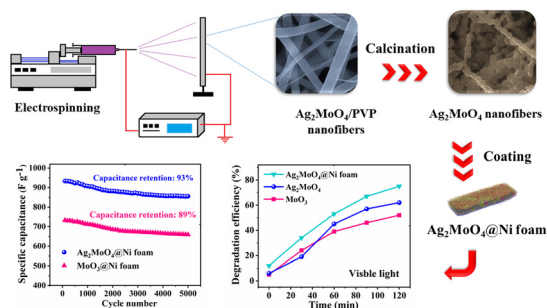
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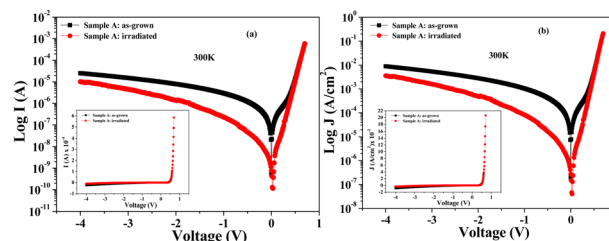
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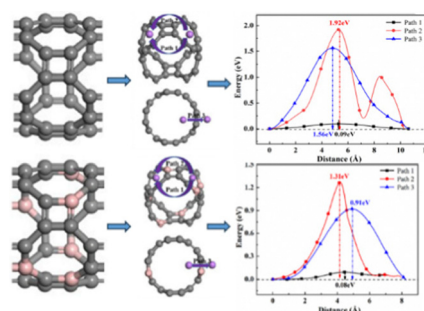
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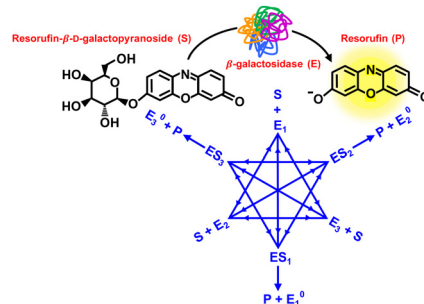
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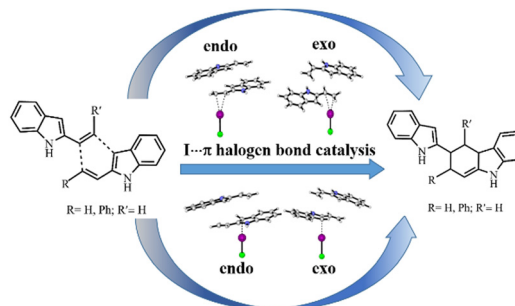
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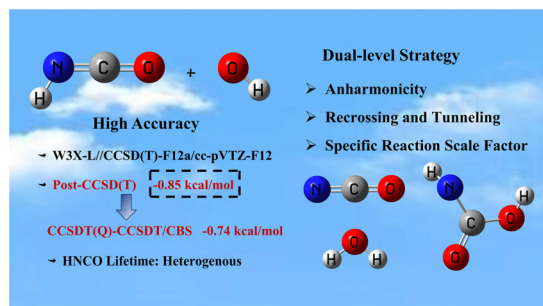
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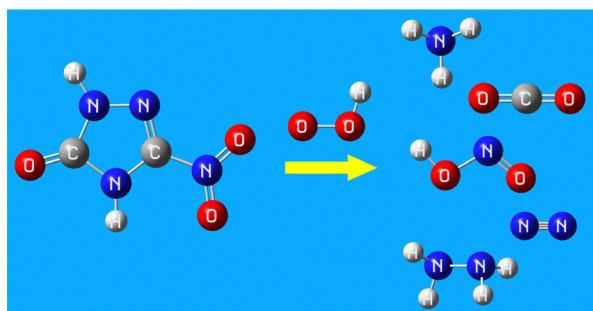
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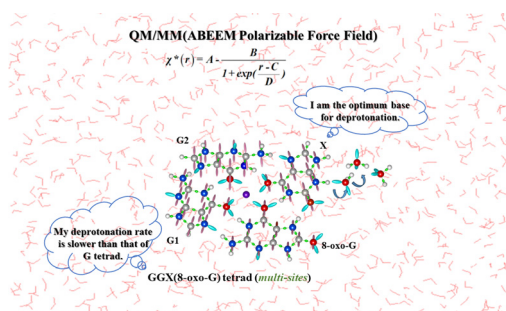
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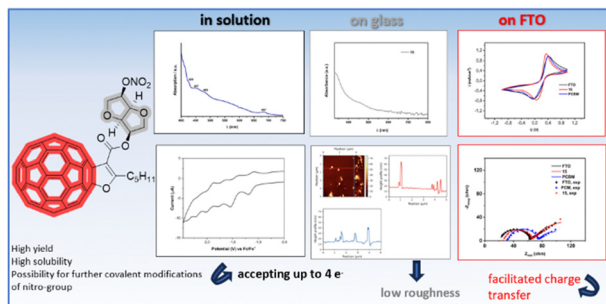
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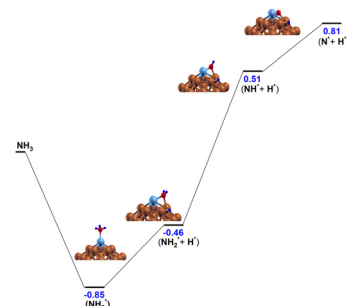


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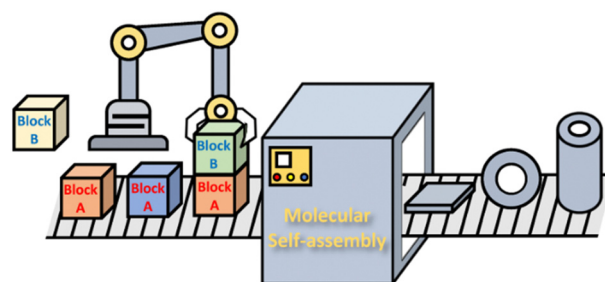
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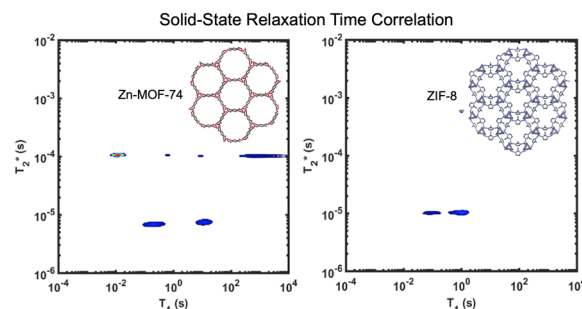
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### *In situ* monitoring of mechanochemical MOF formation by NMR relaxation time correlation

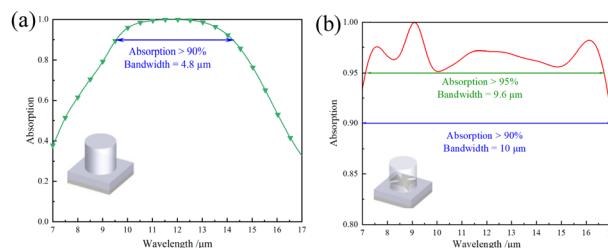
Madeleine E. Leger, Jiangfeng Guo, Bryce MacMillan, Hatem M. Titi, Tomislav Friščić, Bruce Balcom\* and Barry A. Blight\*



551

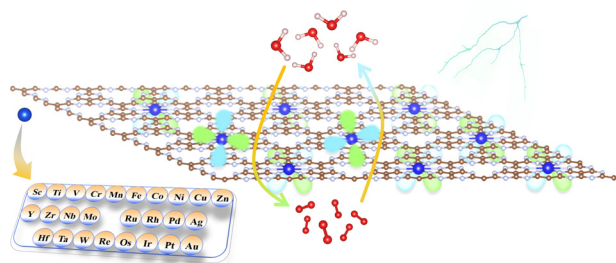
### Design of metamaterial perfect absorbers in the long-wave infrared region

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



## RESEARCH PAPERS

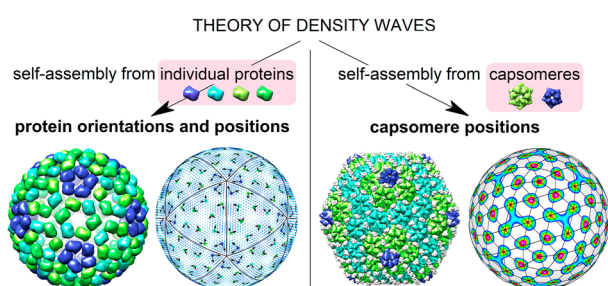
558



### The regulatory function of the d-orbital structure in TM@t-C<sub>4</sub>N<sub>3</sub> for bifunctional catalysis of the oxygen evolution/reduction reaction

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

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

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

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$$rm_0A + m_0B = \frac{1}{u} \{A_{rm_0}B_{m_0}\}_u$$

$$K_{I,m} = \frac{[A]^{rm}[B]^m}{[A_{rm}B_m]} \quad K_{II,m} = [A]^{rm}[B]^m \cdot [A_{rm}B_m]$$

$$u \left( \frac{m}{m_0} \right)^d = 1 \quad (m \leq m_0)$$

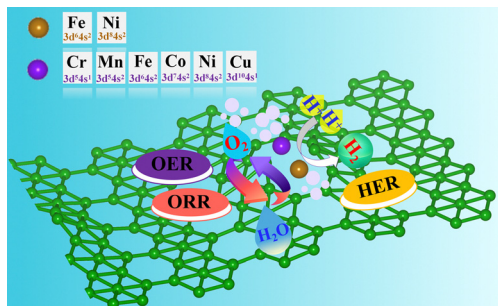
$$K_{I,u} = \frac{[A]^{rm_0}[B]^{m_0}}{[A_{rm_0}B_{m_0}]^{1/u}} \quad K_{II,u} = [A]^{rm_0}[B]^{m_0} \cdot [A_{rm_0}B_{m_0}]^{1/u}$$

$$K_{d,u} = [A]^{rm_0}[B]^{m_0} \quad (u \rightarrow \infty)$$

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

Tian-Lan Zhang

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### Bifunctional diatomic site catalysts supported by $\beta_{12}$ -borophene for efficient oxygen evolution and reduction reactions

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

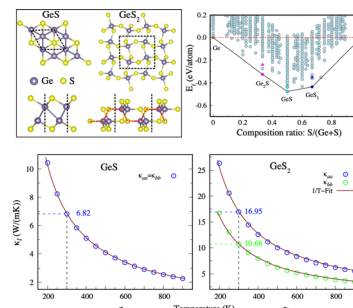


## RESEARCH PAPERS

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# Prediction of novel ground-state structures and analysis of phonon transport in two-dimensional $\text{Ge}_x\text{S}_y$ compounds

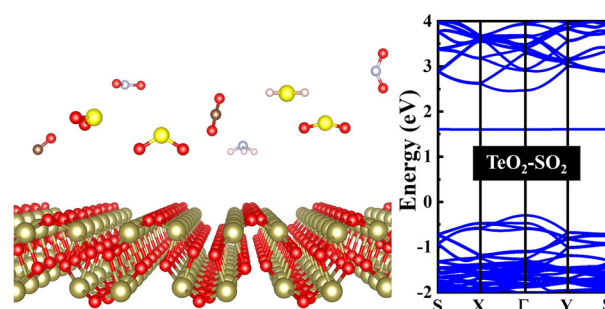
Asad Ali and Young-Han Shin\*



612

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

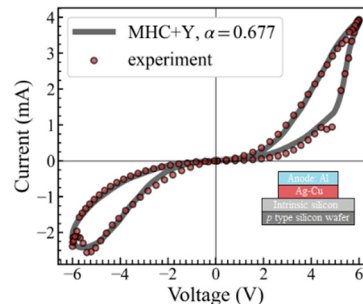
Ying Wang, Shiyong Guo,\* Xiaoyong Xu, Jing Pan, Jingguo Hu and Shengli Zhang\*



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

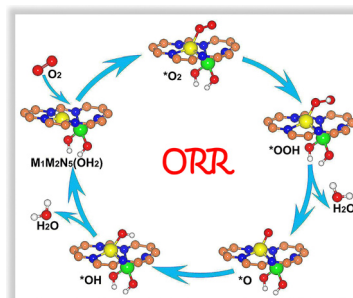
G. V. Paradezhenko,\* D. V. Prodan, A. A. Pervishko, D. Yudin and A. Allagui



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

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**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\*

