

# PCCP

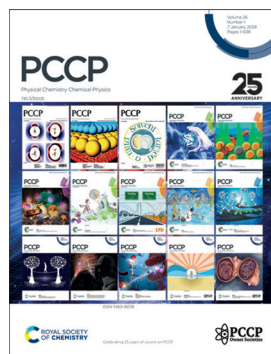
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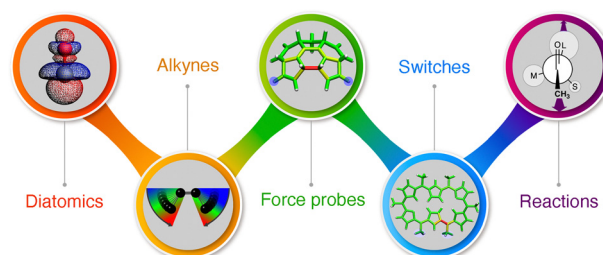
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See Nikola Bregović *et al.*, pp. 67–75. Image reproduced by permission of Nikola Bregović from *Phys. Chem. Chem. Phys.*, 2024, 26, 67.

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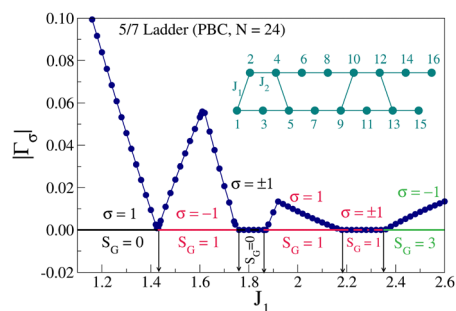
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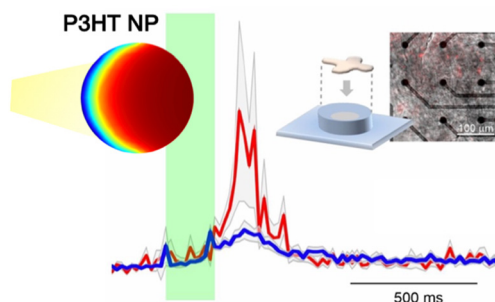


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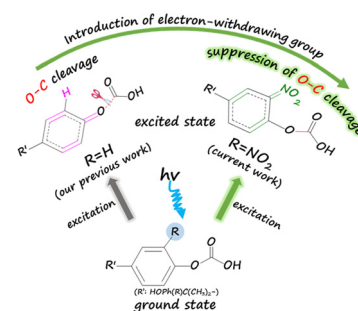
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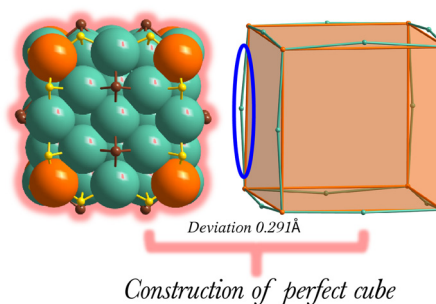
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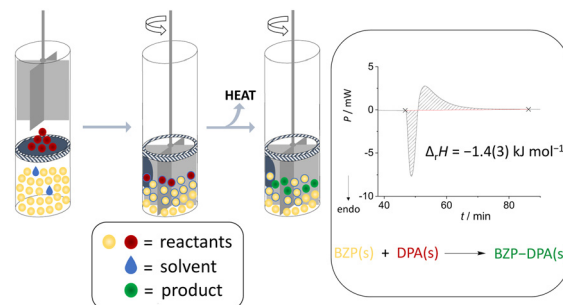


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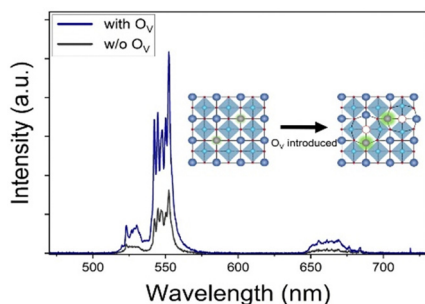
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Marija Cvetnić, Robert Šplajt, Edi Topić, Mirta Rubčić and Nikola Bregović\*



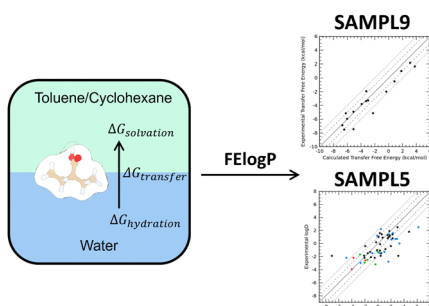
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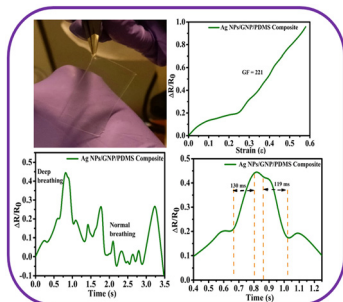
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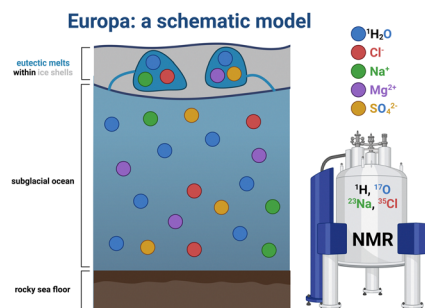
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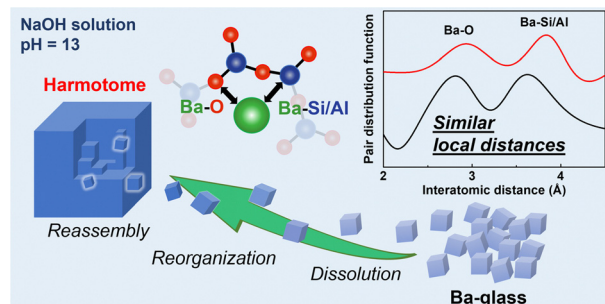




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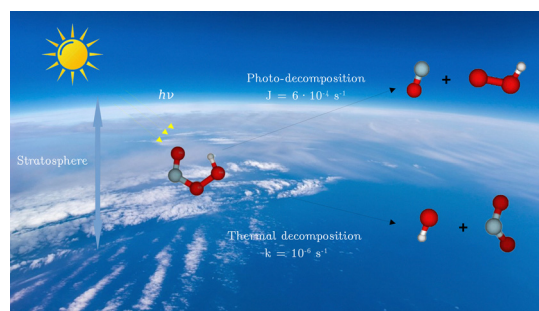
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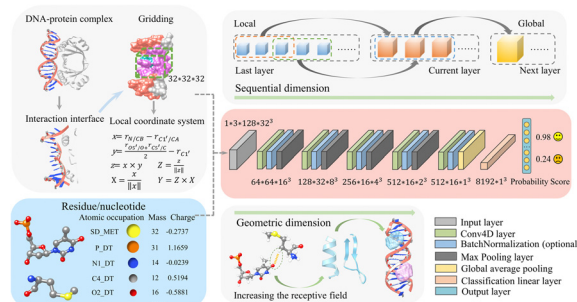
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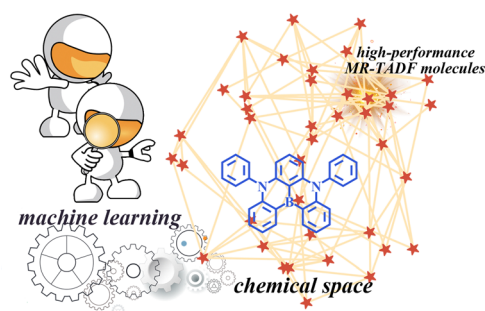
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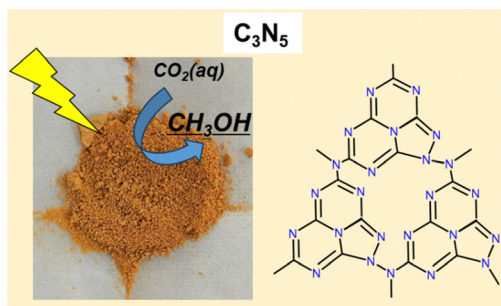
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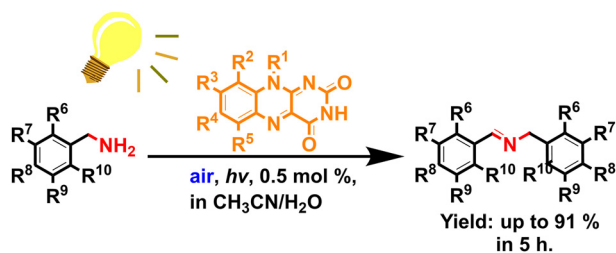
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Kosei Ito and Kei Noda\*

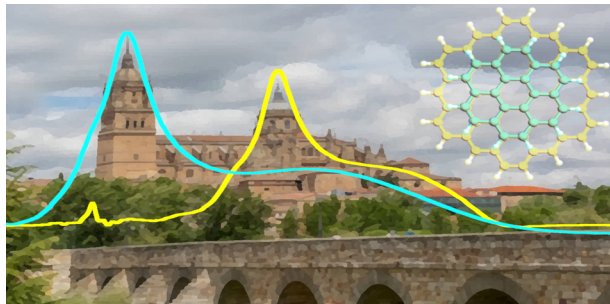
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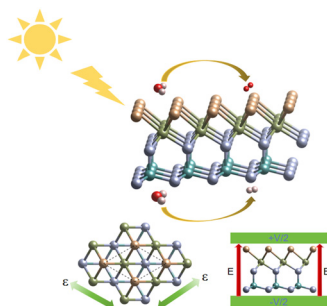
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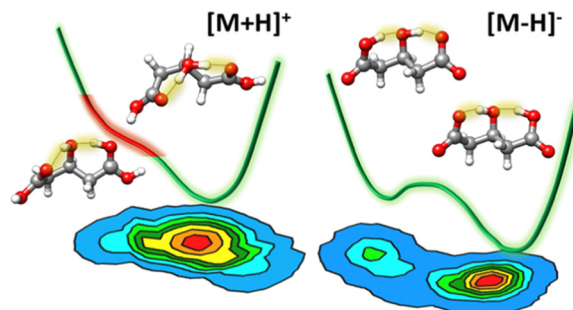


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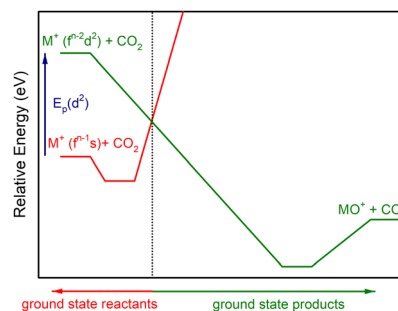
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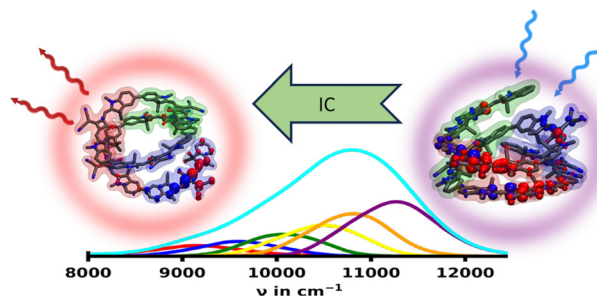
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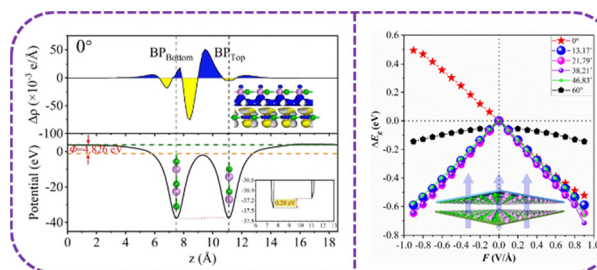
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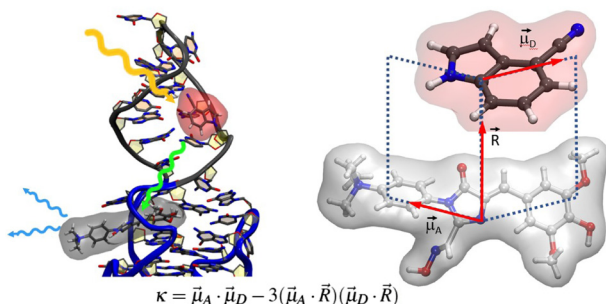
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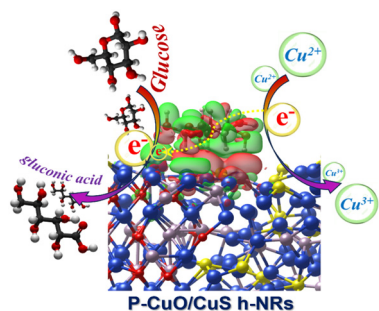
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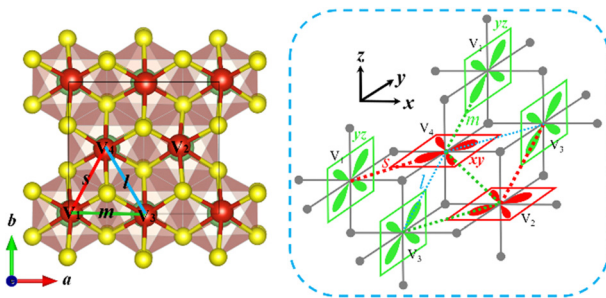
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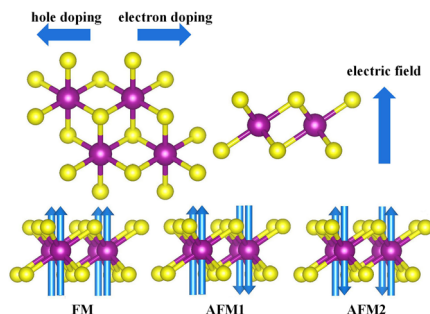
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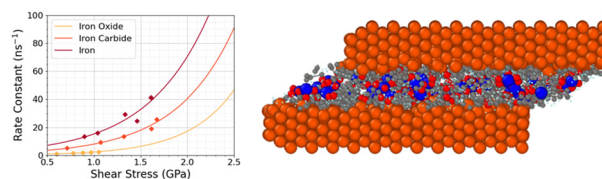




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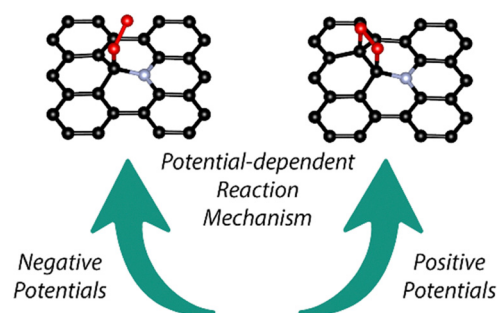
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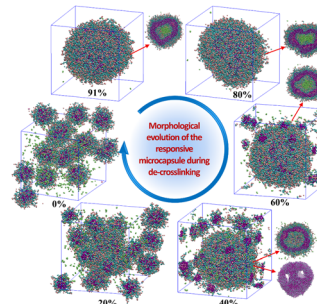
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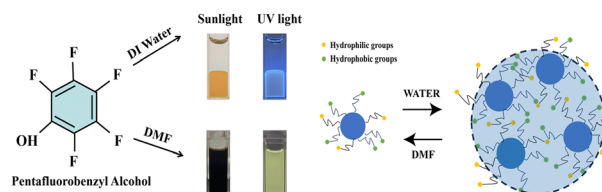
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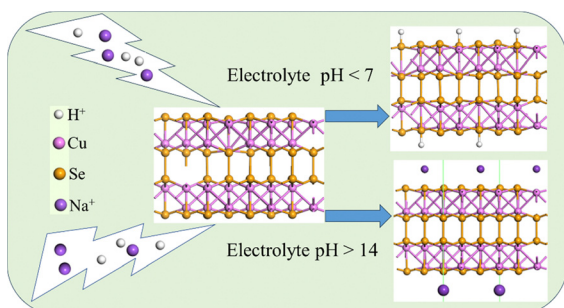
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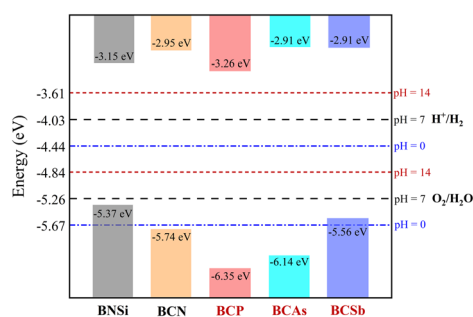
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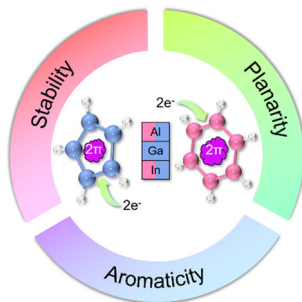
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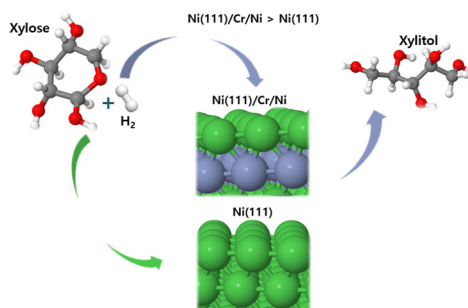
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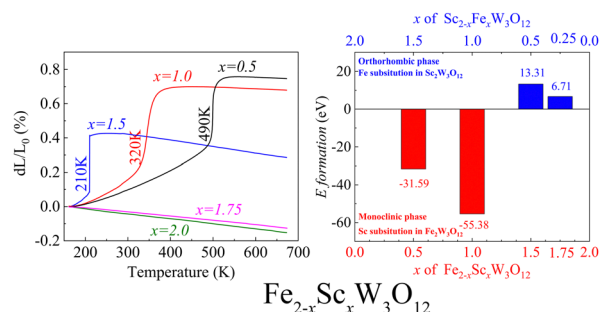


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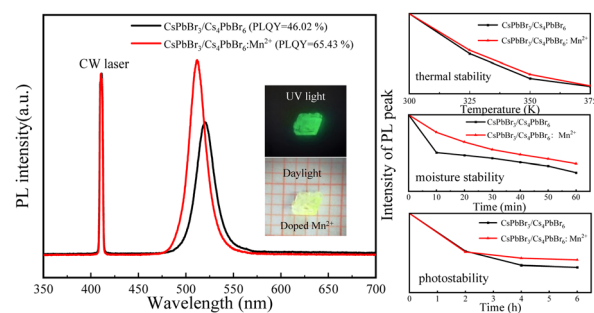
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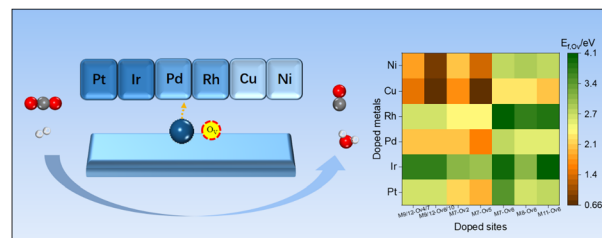
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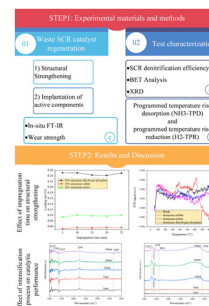
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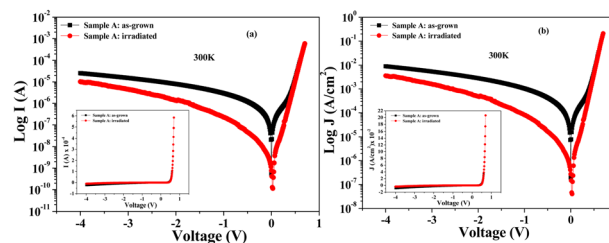


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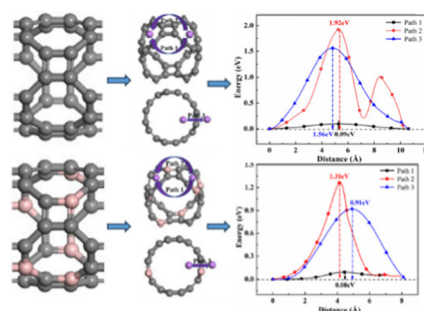
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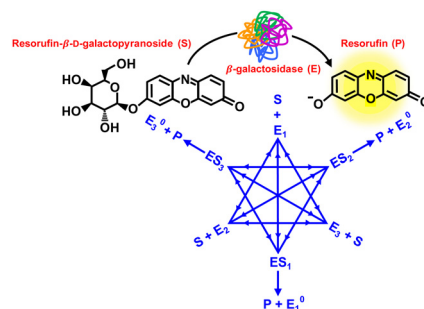
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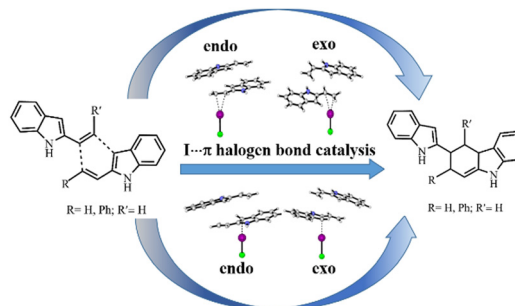
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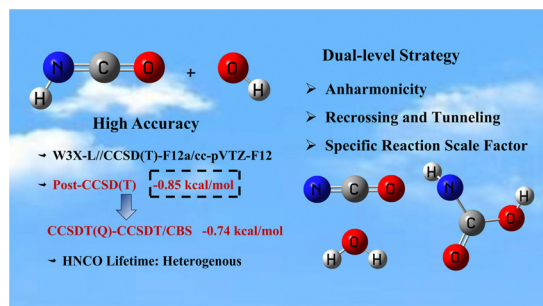
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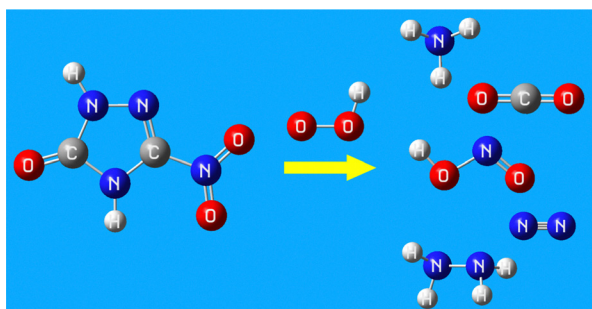
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**Quantitative kinetics of the atmospheric reaction between isocyanic acid and hydroxyl radicals: post-CCSD(T) contribution, anharmonicity, recrossing effects, torsional anharmonicity, and tunneling**

Dai-Dan Deng and Bo Long\*

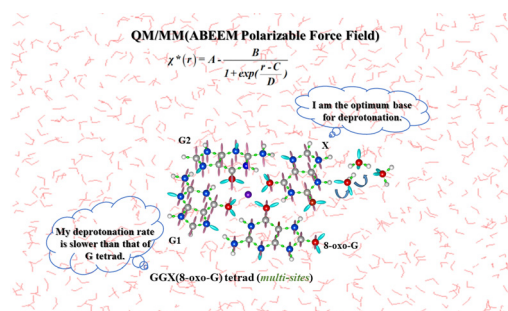
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**Degradation of NTO induced by superoxide and hydroperoxyl radicals: a comprehensive DFT study**

Liudmyla K. Sviatenko, Leonid Gorb and Jerzy Leszczynski\*

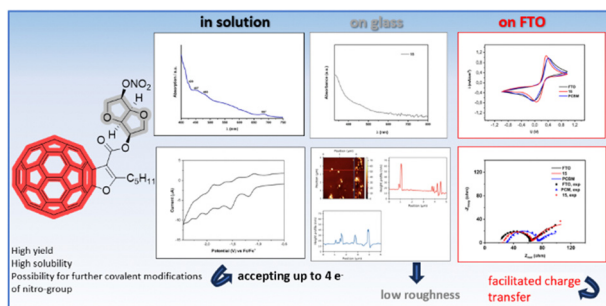
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**Exploring fullerene derivatives for optoelectronic applications: synthesis and characterization study**

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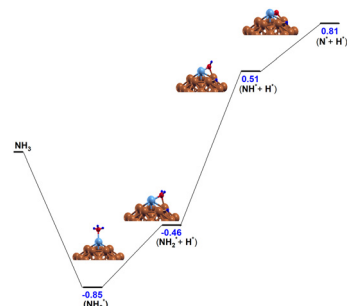




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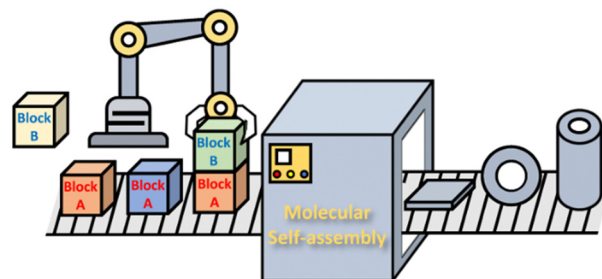
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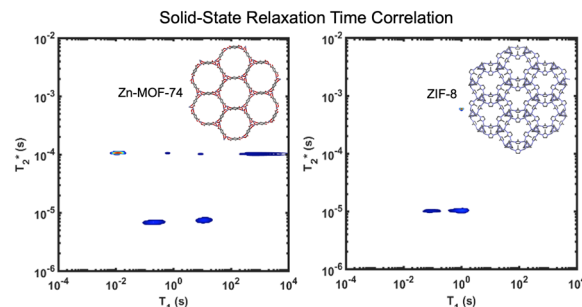
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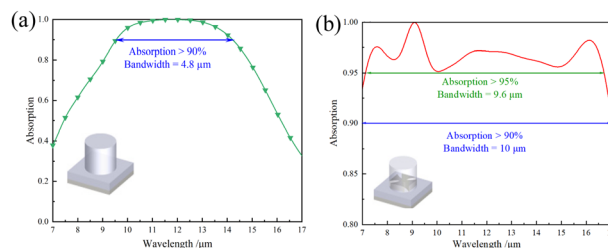
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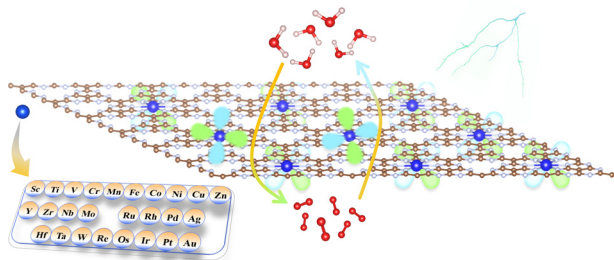
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Yang Wang, Xiu Li, Shenbing Wu, Changjun Hu and Yuanyuan Liu\*



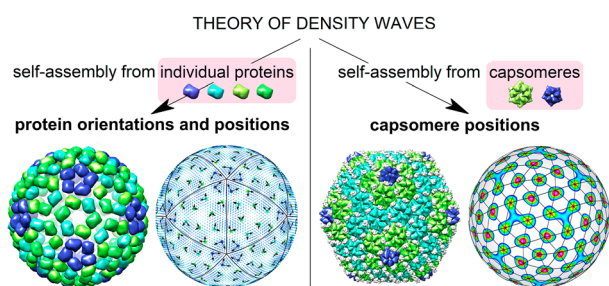
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### The regulatory function of the d-orbital structure in TM@t-C<sub>4</sub>N<sub>3</sub> for bifunctional catalysis of the oxygen evolution/reduction reaction

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

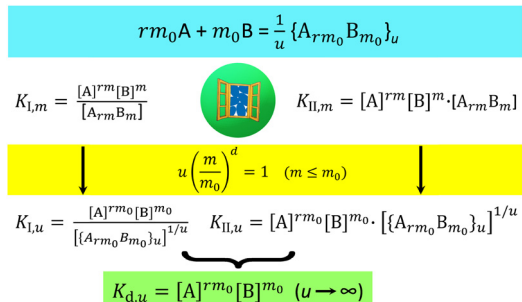
569



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

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

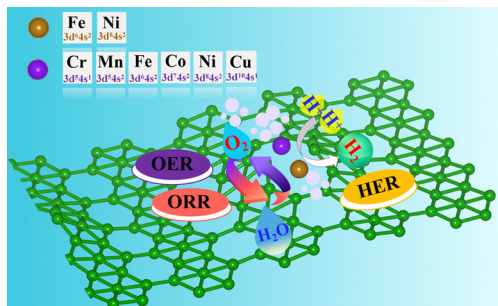
581



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

Tian-Lan Zhang

594



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

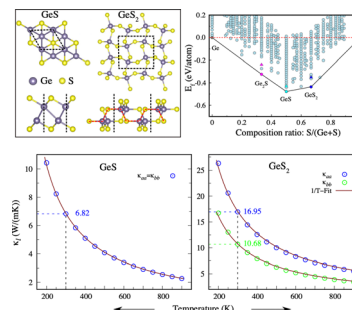
Jia Liu, Minjing Zhang, Si-Dian Li\* and Yuewen Mu\*



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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

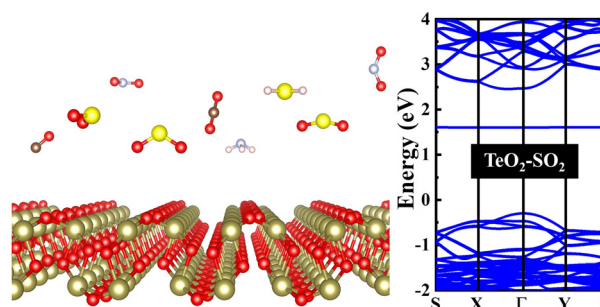
Asad Ali and Young-Han Shin\*



612

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

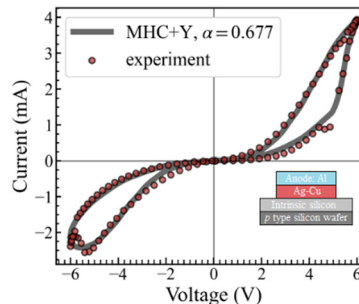
Ying Wang, Shiyong Guo,\* Xiaoyong Xu, Jing Pan, Jingguo Hu and Shengli Zhang\*



621

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

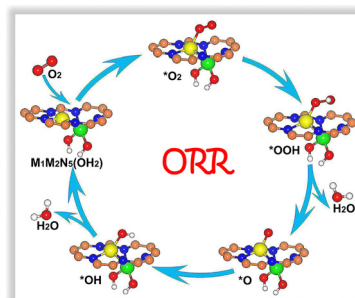
G. V. Paradezhenko,\* D. V. Prodan, A. A. Pervishko, D. Yudin and A. Allagui



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## 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\*

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