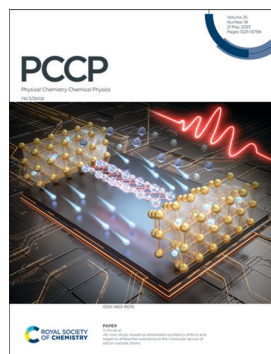


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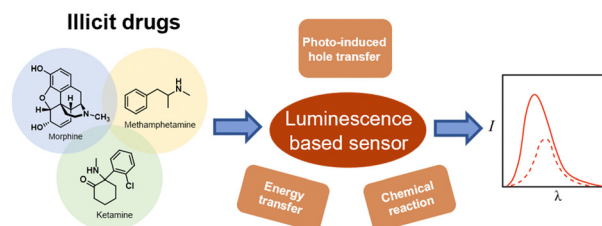


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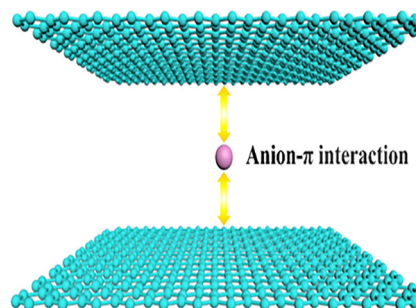


## COMMUNICATION

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**An anomalous anion transfer order in graphene oxide membranes induced by anion- $\pi$  interactions**

Junjie Chen, Jie Li, Xing Liu, Zhenglin He and Guosheng Shi\*

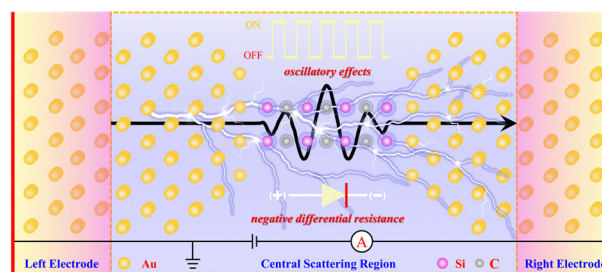


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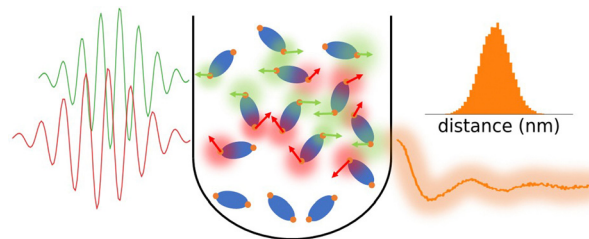
Yi Mu,\* Jie Yu, Rui Hu, Cui-Hong Wang, Cai Cheng and Bang-Pin Hou



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**Efficient sampling of molecular orientations for Cu(II)-based DEER on protein labels**

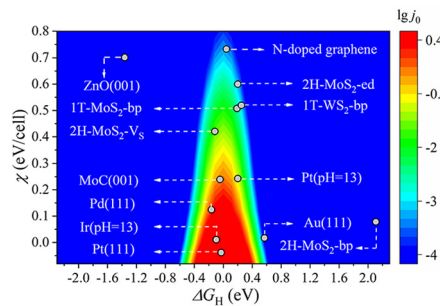
Zikri Hasanbasri, Nicholas A. Moriglioni and Sunil Saxena\*



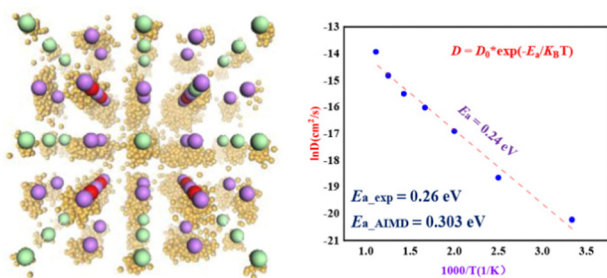
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**Electronegativity principle for hydrogen evolution activity using first-principles calculations**

Yi An, Min Ouyang, Shaoyu Kong, Guangjin Wang and Xiaobo Chen\*



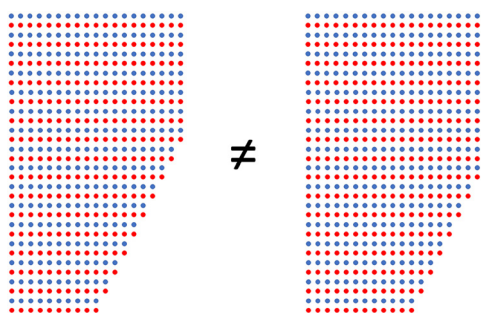
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### Li ion diffusion behavior of $\text{Li}_3\text{OCl}$ solid-state electrolytes with different defect structures: insights from the deep potential model

Zhou Zhang, Zhongyun Ma\* and Yong Pei\*

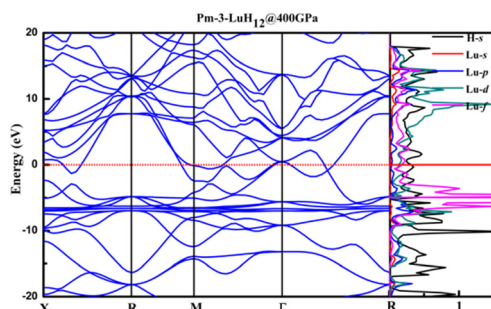
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### The shape effect and its consequences for polar surfaces and for heterogeneous catalysis

Michael Springborg,\* Meijuan Zhou and Bernard Kirtman

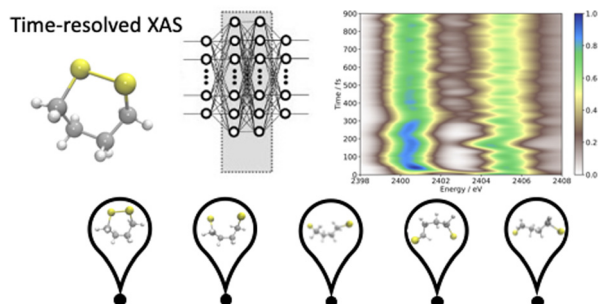
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### Pressure-induced stability and superconductivity in $\text{LuH}_{12}$ polyhydrides

Junyi Du, Weiguo Sun, Xiaofeng Li and Feng Peng\*

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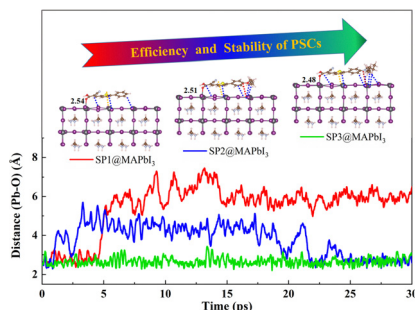
### An on-the-fly deep neural network for simulating time-resolved spectroscopy: predicting the ultrafast ring opening dynamics of 1,2-dithiane

Clelia Middleton, Conor D. Rankine and Thomas J. Penfold\*





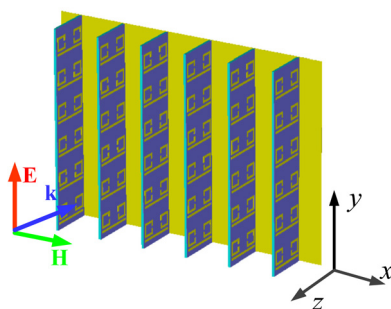
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### Cooperative multiple interactions of donor- $\pi$ -acceptor dyes enhance the efficiency and stability of perovskite solar cells

Xiufang Hou,\* Weiyi Zhang and Quan-Song Li\*

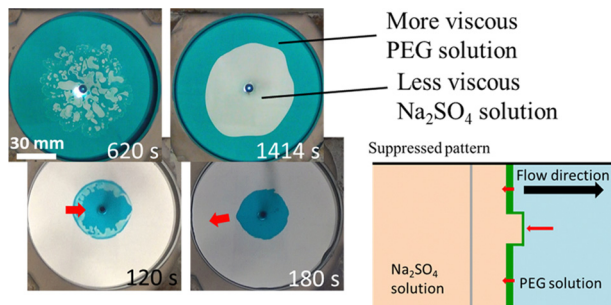
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### Tunable and three-dimensional dual-band metamaterial absorber based on electromagnetically induced transparency with vanadium dioxide

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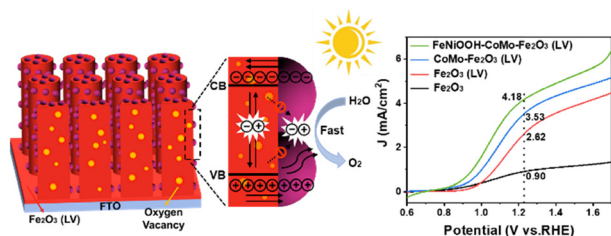
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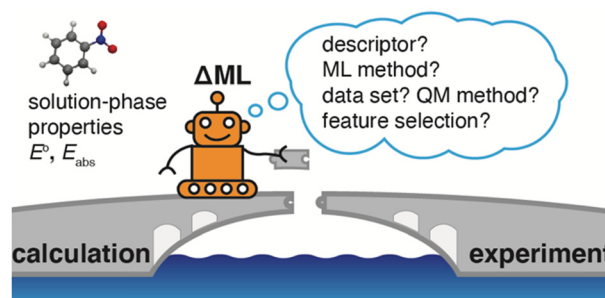
Gaoteng Zhang, Cheng Lu, Chang Li, Shuo Li, Xiaoquan Zhao, Kaiqi Nie, Jiaou Wang, Kun Feng\* and Jun Zhong\*



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### $\Delta$ -Machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states

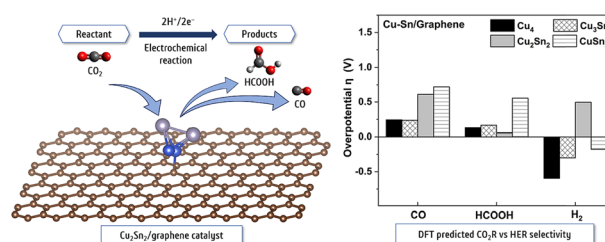
Xu Chen, Pinyuan Li, Eugen Hruska and Fang Liu\*



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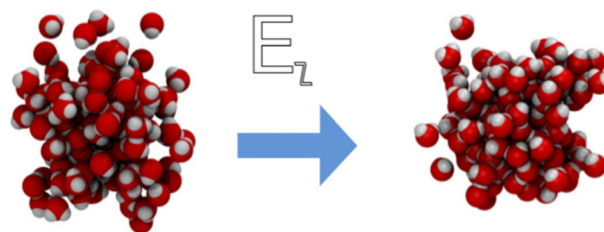
Akshayini Muthuperiyanyagam, Azeem Ghulam Nabi, Qi Zhao, Aman-ur-Rehman and Devis Di Tommaso\*



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### Vibrational dynamics of liquid water in an external electric field

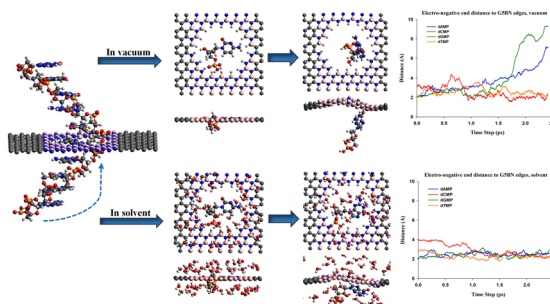
Deepak Ojha\* and Thomas D. Kühne



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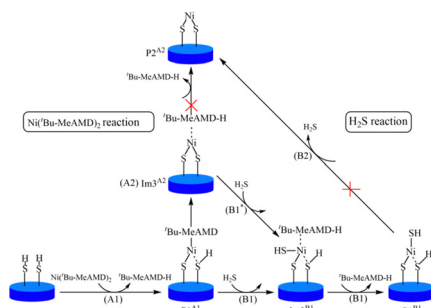
### Exploring the dynamics of DNA nucleotides in graphene/h-BN nanopores: insights from *ab initio* molecular dynamics

Ali Kiakojouri, Irmgard Frank and Ebrahim Nadimi\*



## RESEARCH PAPERS

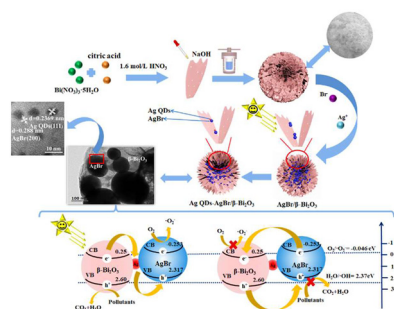
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### Reaction mechanism of nickel sulfide atomic layer deposition using bis(*N,N'*-di-*tert*-butylacetamidinato)nickel(II) and hydrogen sulfide

Xu Zhang, Zhongchao Zhou, Rui Xu, Jiayi Guo, Lina Xu,\*  
Yihong Ding, Hongping Xiao, Xinhua Li, Aidong Li and  
Guoyong Fang\*

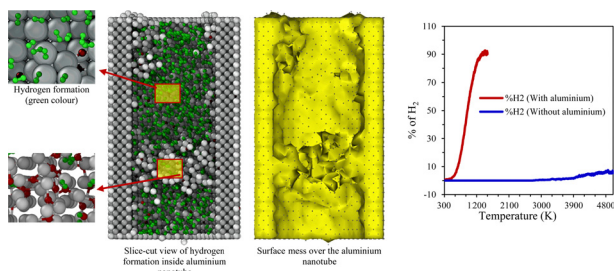
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### Construction of a Z-scheme heterojunction bifunctional photocatalyst with Ag-modified AgBr embedded in $\beta$ - $\text{Bi}_2\text{O}_3$ flowers

Xin Guan, Xiao-li Wang, Xue-wen Zhu, Hui Yu,\*  
Ming Yang, Xiang-ting Dong,\* Ying Yang\* and Long Xia\*

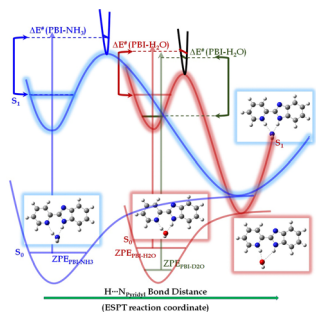
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### Aluminum nanotubes as an efficient catalyst for hydrogen production via thermochemical water splitting: a reactive molecular dynamics simulation

Sunil Kumar\* and Ranjan K. Sahu

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### Excited-state deactivation via solvent-to-chromophore proton transfer in an isolated 1:1 molecular complex: experimental validation by measuring the energy barrier and kinetic isotope effect

Saurabh Khodia, Ramesh Jarupula, Simran Baweja,  
Muhammed Shabeeb, Bhavika Kalal and Surajit Maity\*

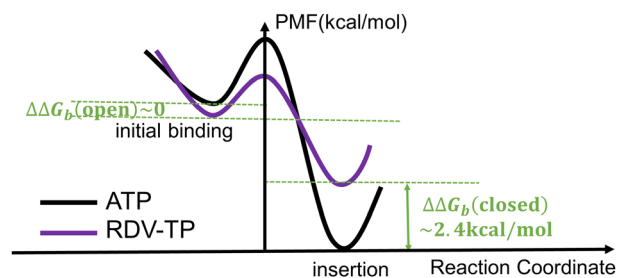


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### Energetic vs. entropic stabilization between a Remdesivir analogue and cognate ATP upon binding and insertion into the active site of SARS-CoV-2 RNA dependent RNA polymerase

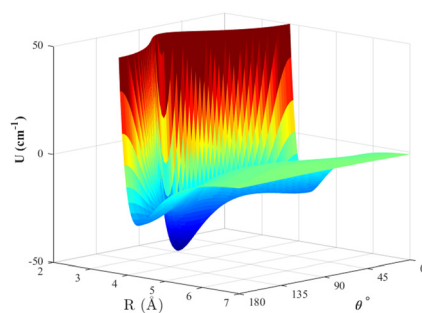
Chunhong Long, Moises Ernesto Romero, Liqiang Dai and Jin Yu\*



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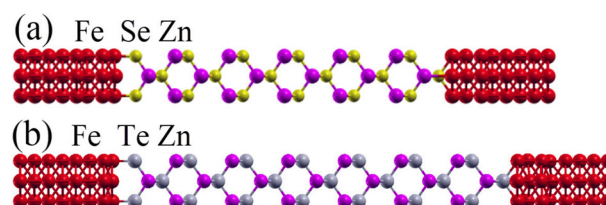
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### ZnSe and ZnTe as tunnel barriers for Fe-based spin valves

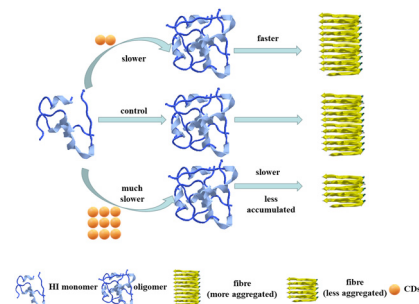
Gokaran Shukla, Hasan M. Abdullah, Avijeet Ray, Shubham Tyagi, Aurélien Manchon, Stefano Sanvito and Udo Schwingenschlögl\*



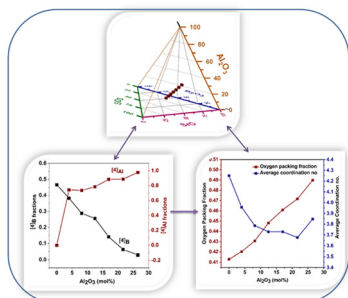
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### Regulation mechanism of human insulin fibrillation by L-lysine carbon dots: low concentration accelerates but high concentration inhibits the fibrillation process

Xing-Yu Liu, Shuai-Chen Du, Feng-Lei Jiang, Peng Jiang\* and Yi Liu\*



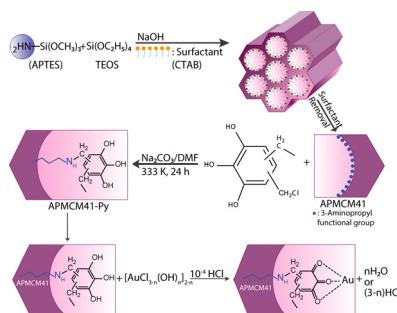
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### An investigation of $\text{Al}_2\text{O}_3$ induced variations in the structural parameters in strontium borosilicate glasses using solid state NMR

Kavya Illath, Prasanta K. Ojha, Sangram K. Rath and T. G. Ajithkumar\*

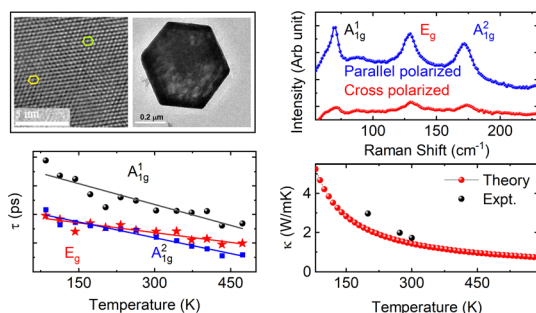
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### Optimization of Au(III) adsorption by the Taguchi method using pyrogallol functionalized silica nanoparticles

Mustafa Can,\* Engin Deniz Parlar, Mustafa Akçil, Abdülkadir Kızıllarlan, Semra Boran, Abdullah Hulusi Kökçam and Özer Uygun

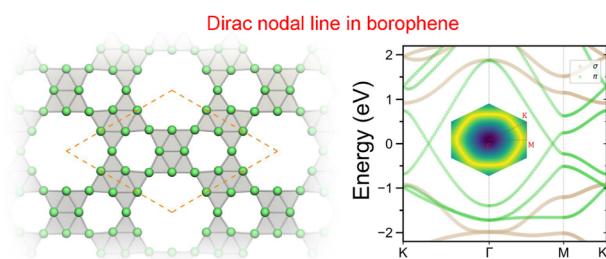
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### Lattice thermal conductivity of topological insulator $\text{Bi}_2\text{Se}_3$ nanocrystals: comparison from theoretical and experimental

Vipin K. E., Soumendra Kumar Das and Prahallad Padhan\*

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### A two-dimensional borophene monolayer with ideal Dirac nodal-line fermions

Chengyong Zhong,\* Xuelian Li, Chunbao Feng and Peng Yu\*

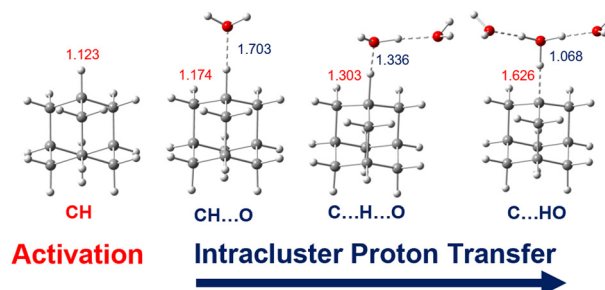


## RESEARCH PAPERS

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### Microhydration of the adamantane cation: intracuster proton transfer to solvent in $[\text{Ad}(\text{H}_2\text{O})_{n=1-5}]^+$ for $n \geq 3$

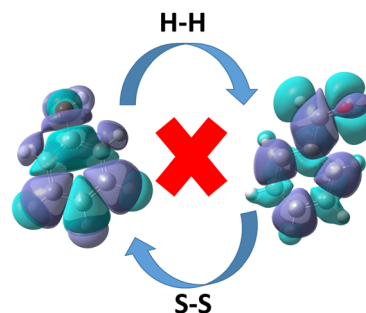
Martin Andreas Robert George and Otto Dopfer\*



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### Can we predict ambident regioselectivity using the chemical hardness?

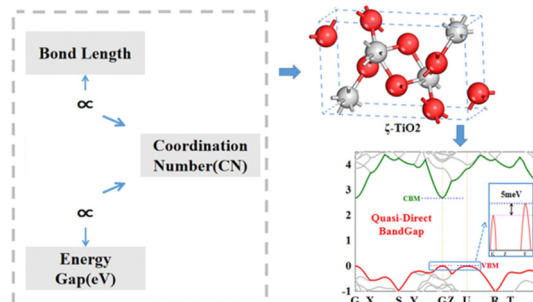
Ramón Alain Miranda-Quintana,\* Alberto Vela, Frank De Proft, Marco Martínez González and José L. Gázquez



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### Novel three-dimensional $\text{TiO}_2$ structure with a unique quasi-direct band gap for photocatalysts

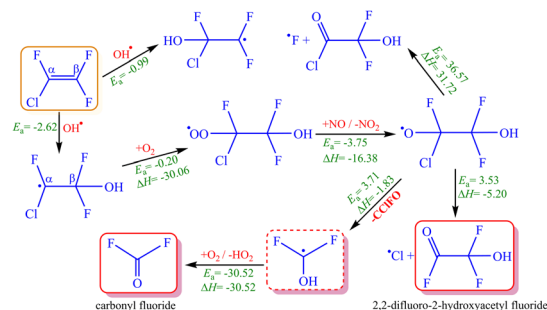
Jiayi Guo, Wangping Xu, Juexian Cao\* and Xiaolin Wei\*



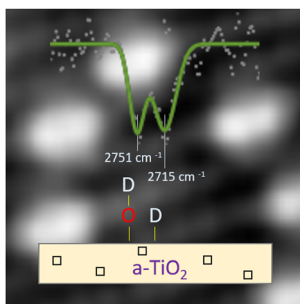
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### Understanding the kinetics and atmospheric degradation mechanism of chlorotrifluoroethylene ( $\text{CF}_2=\text{CFCl}$ ) initiated by OH radicals

Saber Safari Balsini, Abolfazl Shiroudi,\* Farhad Hatamjafari,\* Ehsan Zahedi, Khalil Pourshamsian and Ahmad Reza Oliaey



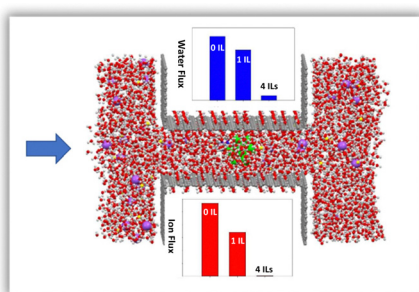
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### Origin of hydroxyl pair formation on reduced anatase TiO<sub>2</sub>(101)

Kræn C. Adamsen, Nikolay G. Petrik,\* Wilke Dononelli, Greg A. Kimmel, Tao Xu, Zheshen Li, Lutz Lammich, Bjørk Hammer, Jeppe V. Lauritsen and Stefan Wendt\*

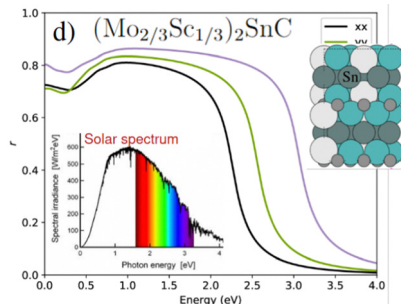
13654



### Polyoxometalate ionic liquid between graphene oxide surfaces as a new membrane in the desalination process: a molecular dynamics study

Mohsen Abbaspour

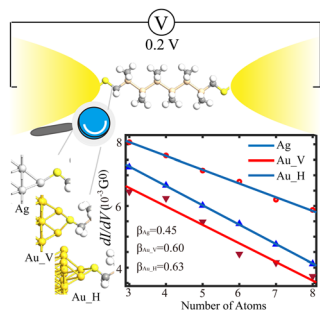
13665



### Optical properties of in-plane chemically ordered *i*-MAX structures

Junais Habeeb Mokkath

13673



### Silver electrodes provide higher conductance than gold for thiol-terminated oligosilane molecular junctions: the interfacial effect

Minglang Wang,\* Xianglin Chen, Wenjun Lu, Xinyue Tian and Guang-Ping Zhang

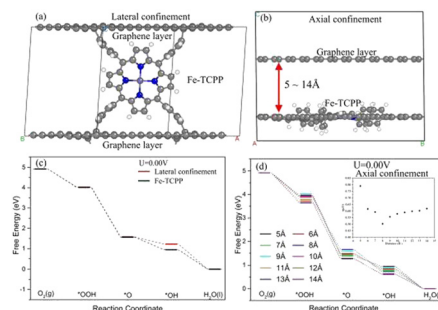


## RESEARCH PAPERS

13683

### Exploration of spatial confinement and ligand effects for the oxygen reduction reaction on Fe–N<sub>x</sub> embedded hole-graphene

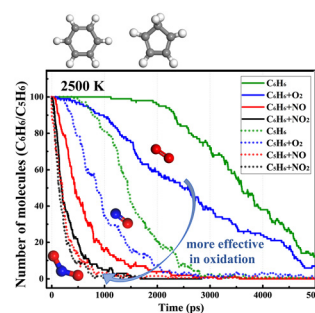
Jing-Hua Guo,\* Hong-Bo Wang, Hai-Ying Liu, Gang Chen\* and Ting-Ting Cao



13690

### Pyrolysis and oxidation of benzene and cyclopentadiene by NO<sub>x</sub>: a ReaxFF molecular dynamics study

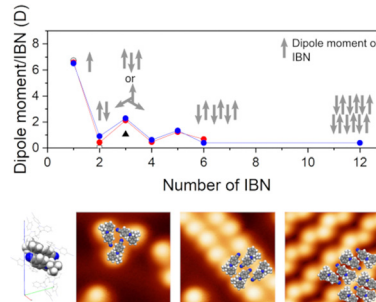
Ying Wang, Lei Zhou, Qian Mao,\* Zhanyuan Wang and Haiqiao Wei\*



13702

### Dipole-moment-induced supramolecular assembly of a donor–acceptor-type molecule on a metal surface and in a crystal

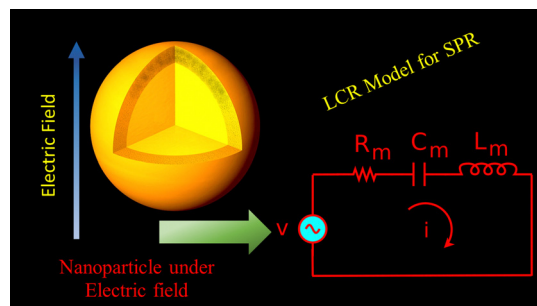
W. Nakanishi,\* Y. Matsushita, M. Takeuchi and K. Sagisaka\*



13708

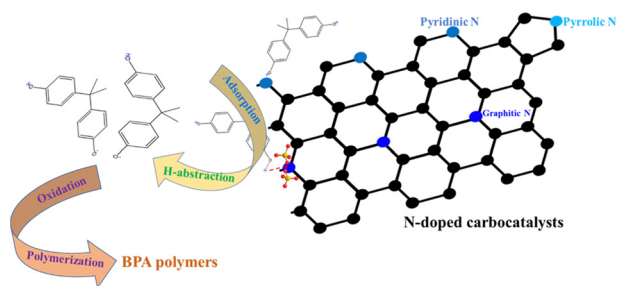
### Surface plasmon resonance in metal nanospheres explained with LCR circuits

Shivangi Dubey, Kuldeep Kumar\* and P. Arun



## RESEARCH PAPERS

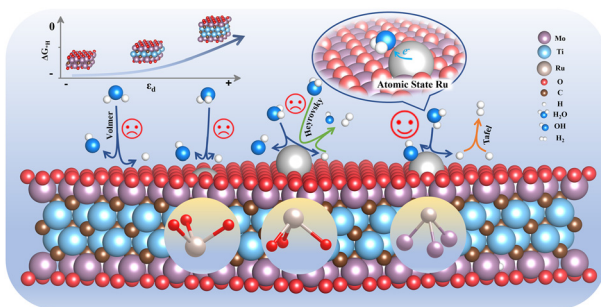
13716



### Nitrogen-doped carbocatalyst activated persulfate (PS) for oxidation polymerization of bisphenol A (BPA): importance of nonradical activation of PS

Caihong Wang, Yong Liu,\* Fengshen Han, Yongzhe Han, Tianyu Liu, Haitao Ren and Xu Han\*

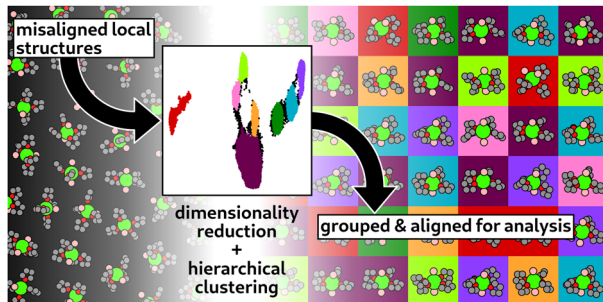
13728



### Single atom supported on MXenes for the alkaline hydrogen evolution reaction: species, coordination environment, and action mechanism

Zijun Sun, Rui Li,\* Qing Xi, Fangxia Xie, Xuan Jian, Xiaoming Gao, Houfen Li, Zhuobin Yu, Jianxin Liu, Xiaochao Zhang, Yawen Wang, Yunfang Wang, Xiuping Yue\* and Caimei Fan

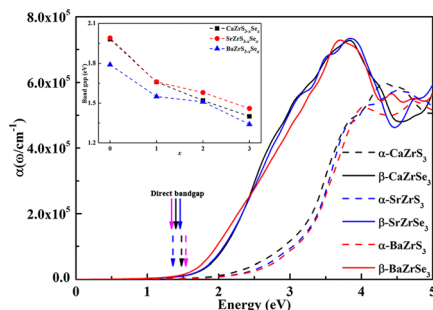
13741



### Unsupervised learning of representative local atomic arrangements in molecular dynamics data

Fabrice Roncoroni, Ana Sanz-Matias, Siddharth Sundararaman and David Prendergast\*

13755



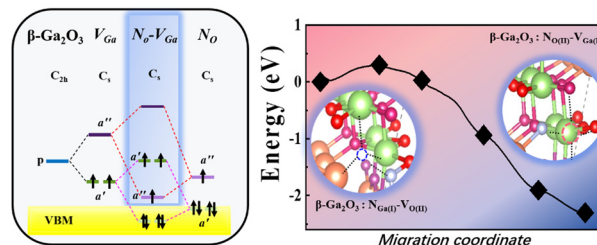
### Computational study of the fundamental properties of Zr-based chalcogenide perovskites for optoelectronics

Diwen Liu,\* Huihui Zeng, Huan Peng and Rongjian Sa\*

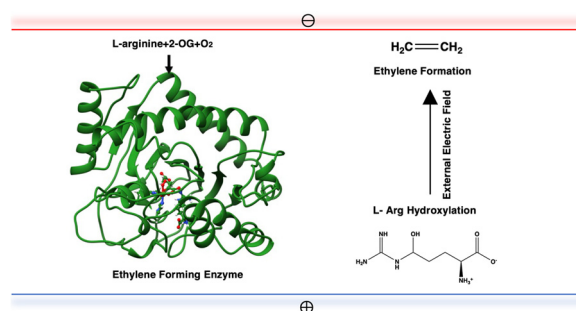


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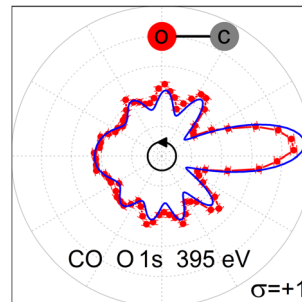
13766

**P-type nitrogen-doped  $\beta$ -Ga<sub>2</sub>O<sub>3</sub>: the role of stable shallow acceptor N<sub>O</sub>-V<sub>Ga</sub> complexes**Congcong Ma, Zhengyuan Wu, Hao Zhang,\*  
Heyuan Zhu, Junyong Kang, Junhao Chu and Zhilai Fang\*

13772

**Can an external electric field switch between ethylene formation and L-arginine hydroxylation in the ethylene forming enzyme?**Shobhit S. Chaturvedi, Simahudeen Bathir  
Jaber Sathik Rifayee, Rajeev Ramanan, Joel A. Rankin,  
Jian Hu, Robert P. Hausinger and Christo Z. Christov\*

13784

**High-energy molecular-frame photoelectron angular distributions: a molecular bond-length ruler**I. Vela-Peréz, F. Ota, A. Mhamdi, Y. Tamura, J. Rist,  
N. Melzer, S. Uerken, G. Nalin, N. Anders, D. You,  
M. Kircher, C. Janke, M. Waitz, F. Trinter,\* R. Guillemin,  
M. N. Piancastelli, M. Simon, V. T. Davis, J. B. Williams,  
R. Dörner, K. Hatada, K. Yamazaki, K. Fehre,  
Ph. V. Demekhin,\* K. Ueda, M. S. Schöffler and T. Jahnke\*

## CORRECTION

13792

**Correction: Crystalline matrix-activated spin-forbidden transitions of engineered organic crystals**

Heming Zhang, Lianbao Ke, Yufang Nie, Zhengqian Tu, Jiaxuan Wang, Semion K. Saikin, Hai Bi\* and Yue Wang

