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ISSN 1463–9076 CODEN PPCPFQ 25(19) 13211–13794 (2023)



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### Inside cover

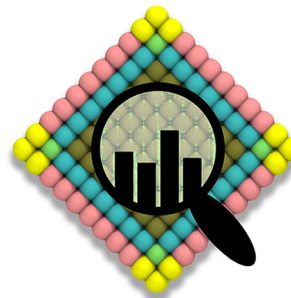
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pp. 13275–13288.  
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*Phys. Chem. Chem. Phys.*,  
2023, 25, 13275.

## TUTORIAL REVIEW

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### *In silico* characterization of nanoparticles

Björn Kirchoff,\* Christoph Jung, Daniel Gaissmaier,  
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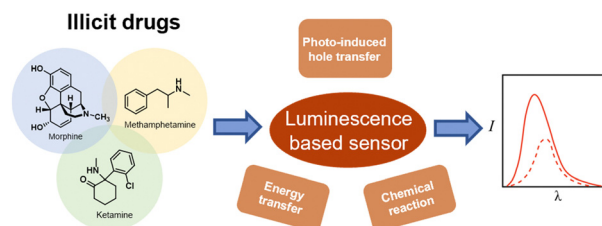


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### Luminescence-based detection and identification of illicit drugs

M. Chen, P. L. Burn\* and P. E. Shaw\*



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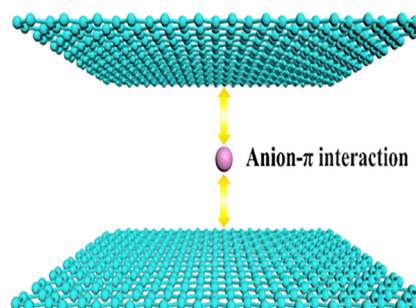


## COMMUNICATION

13260

**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\*

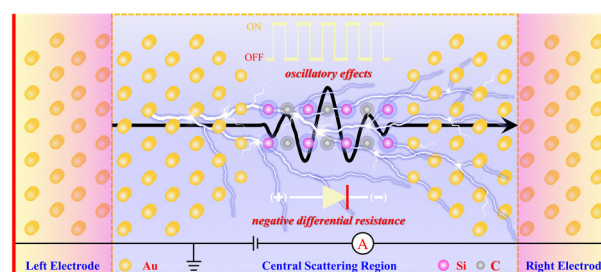


## RESEARCH PAPERS

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**Ab initio study revealing remarkable oscillatory effects and negative differential resistance in the molecular device of silicon carbide chains**

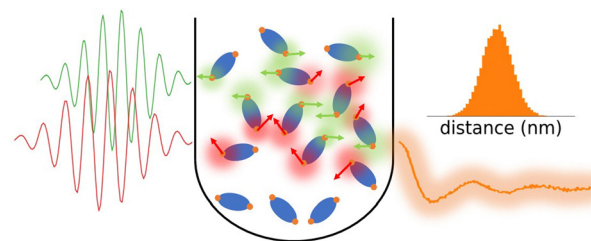
Yi Mu,\* Jie Yu, Rui Hu, Cui-Hong Wang, Cai Cheng and Bang-Pin Hou



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

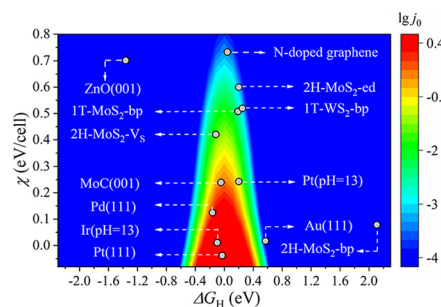
Zikri Hasanbasri, Nicholas A. Moriglioni and Sunil Saxena\*



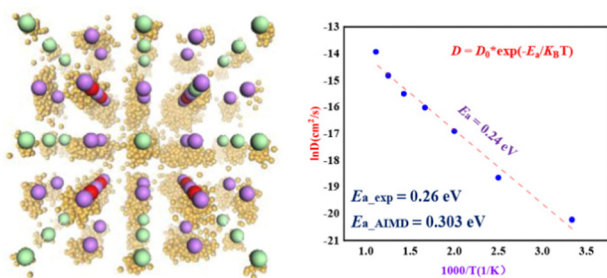
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**Electronegativity principle for hydrogen evolution activity using first-principles calculations**

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



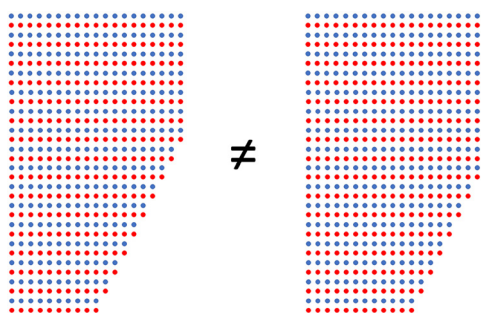
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### Li ion diffusion behavior of $\text{Li}_3\text{OCl}$ solid-state electrolytes with different defect structures: insights from the deep potential model

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

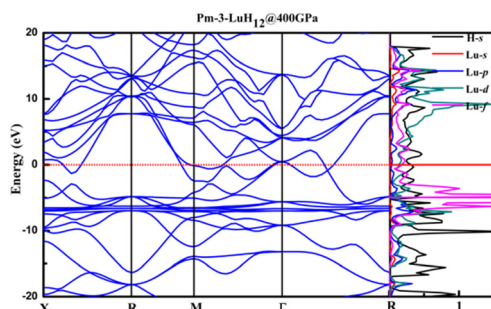
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### The shape effect and its consequences for polar surfaces and for heterogeneous catalysis

Michael Springborg,\* Meijuan Zhou and Bernard Kirtman

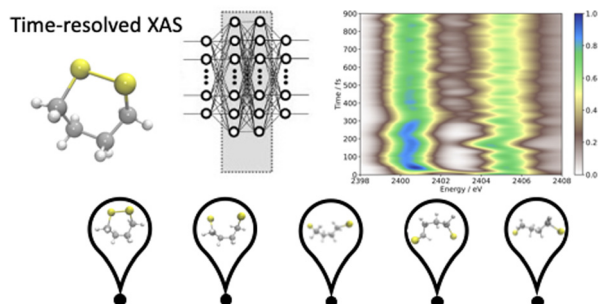
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### Pressure-induced stability and superconductivity in $\text{LuH}_{12}$ polyhydrides

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\*

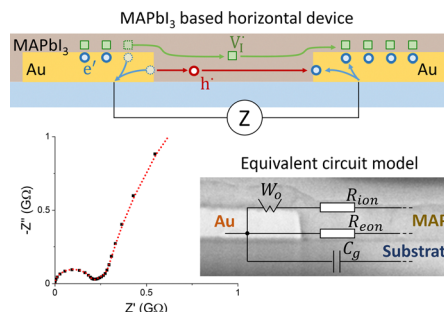


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## Ionic and electronic polarization effects in horizontal hybrid perovskite device structures close to equilibrium

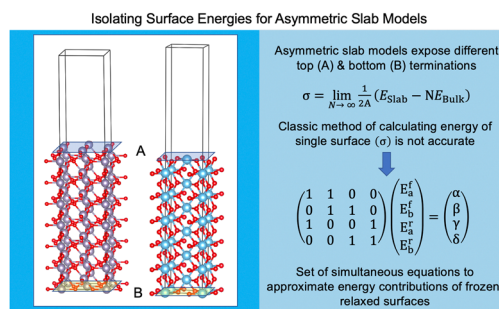
Davide Moia,\* Mina Jung, Ya-Ru Wang and Joachim Maier



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## A method of calculating surface energies for asymmetric slab models

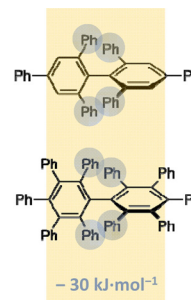
Natalie M. Stuart\* and Karl Sohlberg



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## How great is the stabilization of crowded polyphenylbiphenyls by London dispersion?

Carlos F. R. A. C. Lima, Joel T. Mague, Yuchen Du, Robert A. Pascal Jr and Luís M. N. B. F. Santos\*

Too Crowded or  
not Too Crowded?

Strain | Dispersion Balance

Thermodynamic evidence

Deficient DFT description

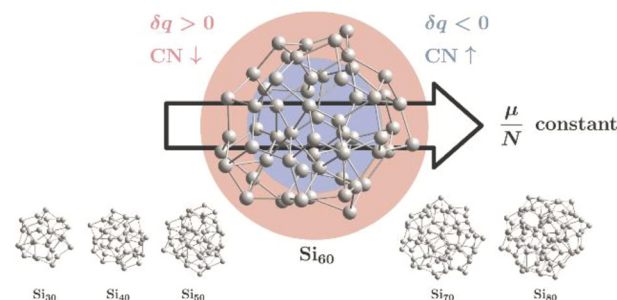
Great stabilization by

London Dispersion

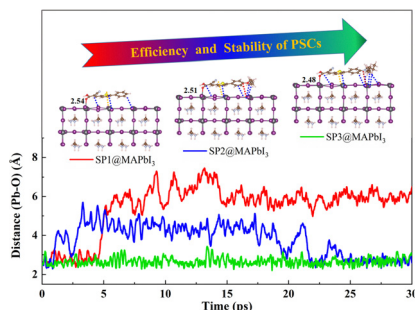
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## Scaling of the permanent electric dipole moment in isolated silicon clusters with near-spherical shape

Filip Rivic,\* Andreas Lehr and Rolf Schäfer



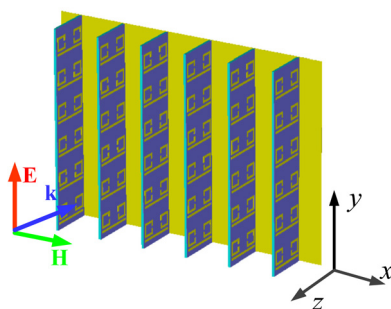
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### Cooperative multiple interactions of donor- $\pi$ -acceptor dyes enhance the efficiency and stability of perovskite solar cells

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

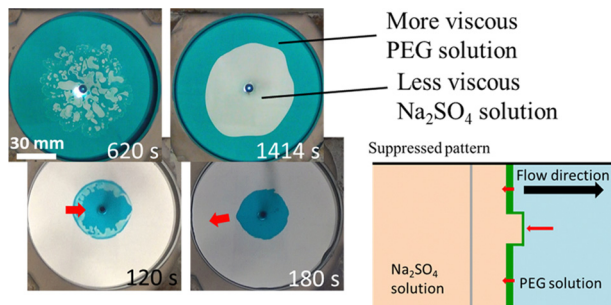
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### Tunable and three-dimensional dual-band metamaterial absorber based on electromagnetically induced transparency with vanadium dioxide

Mingming Chen\* and Xue-Xia Yang\*

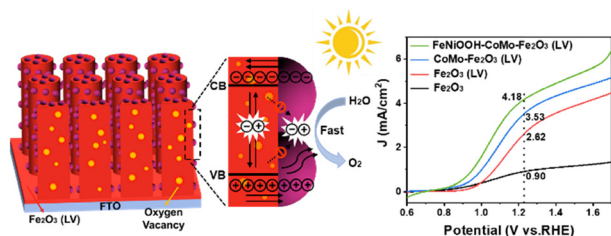
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### Experimental demonstration of the suppression of viscous fingering in a partially miscible system

Kaori Iwasaki, Yuichiro Nagatsu, Takahiko Ban, Jun Iijima, Manoranjan Mishra and Ryuta X. Suzuki\*

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### CoMoO<sub>4</sub>-modified hematite with oxygen vacancies for high-efficiency solar water splitting

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



13417

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

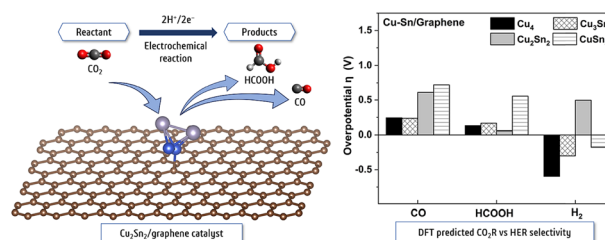
Xu Chen, Pinyuan Li, Eugen Hruska and Fang Liu\*



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### Adsorption, activation, and conversion of carbon dioxide on small copper–tin nanoclusters

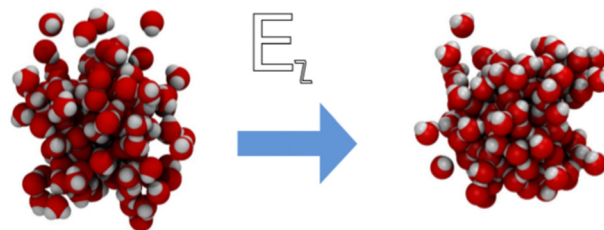
Akshayini Muthuperiyanayagam, Azeem Ghulam Nabi, Qi Zhao, Aman-ur-Rehman and Devis Di Tommaso\*



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

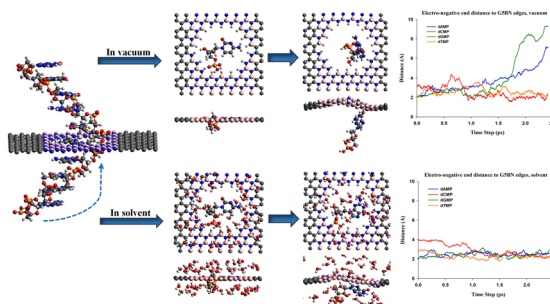
Deepak Ojha\* and Thomas D. Kühne



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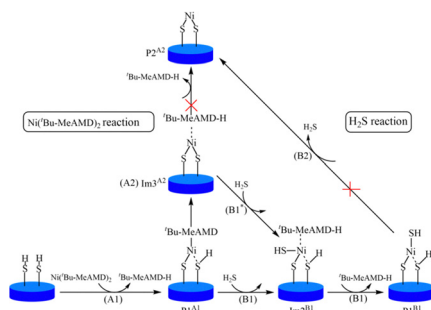
### Exploring the dynamics of DNA nucleotides in graphene/h-BN nanopores: insights from *ab initio* molecular dynamics

Ali Kiakojouri, Irmgard Frank and Ebrahim Nadimi\*



## RESEARCH PAPERS

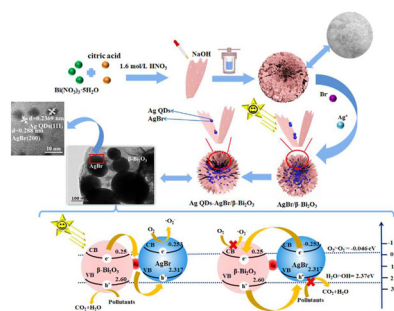
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### Reaction mechanism of nickel sulfide atomic layer deposition using bis(*N,N'*-di-*tert*-butylacetamidinato)nickel(II) and hydrogen sulfide

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

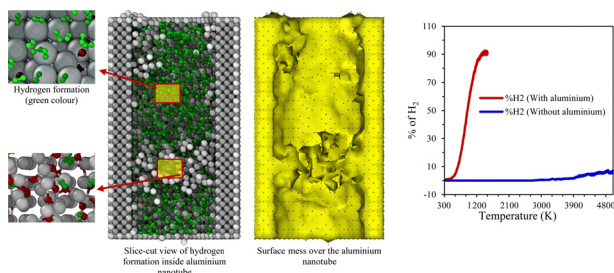
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### Construction of a Z-scheme heterojunction bifunctional photocatalyst with Ag-modified AgBr embedded in $\beta$ - $\text{Bi}_2\text{O}_3$ flowers

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

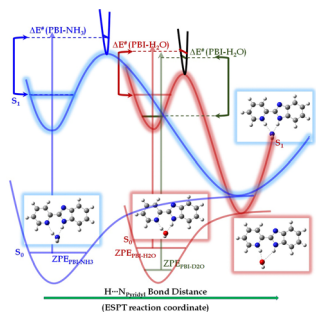
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### Aluminum nanotubes as an efficient catalyst for hydrogen production via thermochemical water splitting: a reactive molecular dynamics simulation

Sunil Kumar\* and Ranjan K. Sahu

13498



### 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\*

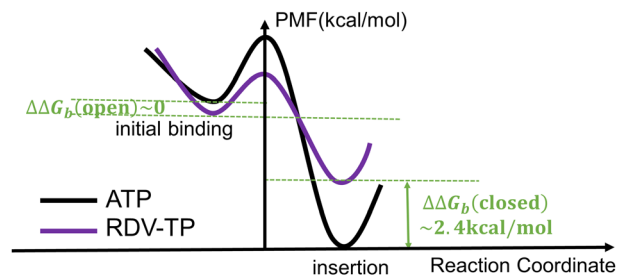


## RESEARCH PAPERS

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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

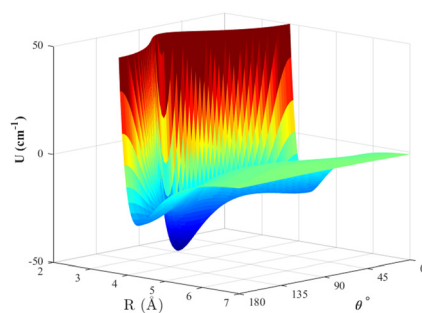
Chunhong Long, Moises Ernesto Romero, Liqiang Dai and Jin Yu\*



13521

### Quantum mechanical and classical calculation of the transport and relaxation properties of He ··· CO<sub>2</sub> complex using a new PES

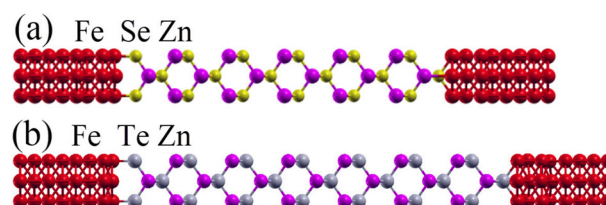
Ebrahim Nemati-Kande,\* Fatemeh Aghababaei and Salar Sadeghi



13533

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

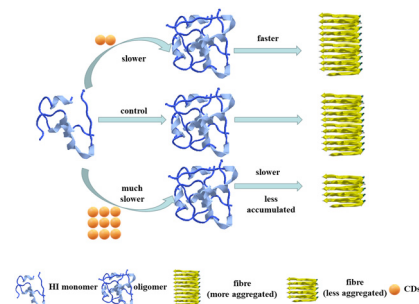
Gokaran Shukla, Hasan M. Abdullah, Avijeet Ray, Shubham Tyagi, Aurélien Manchon, Stefano Sanvito and Udo Schwingenschlögl\*



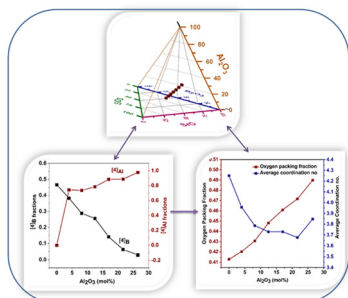
13542

### 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\*



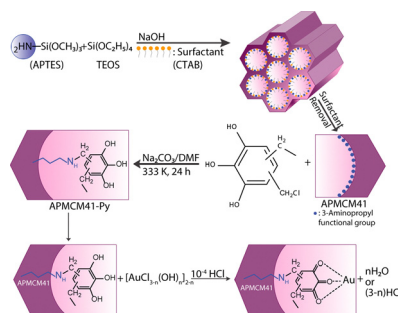
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### An investigation of $\text{Al}_2\text{O}_3$ induced variations in the structural parameters in strontium borosilicate glasses using solid state NMR

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

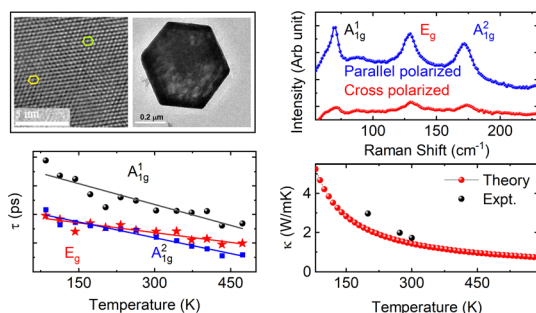
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### Optimization of Au(III) adsorption by the Taguchi method using pyrogallol functionalized silica nanoparticles

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

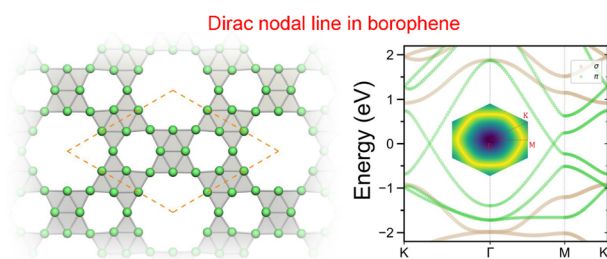
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### Lattice thermal conductivity of topological insulator $\text{Bi}_2\text{Se}_3$ nanocrystals: comparison from theoretical and experimental

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\*

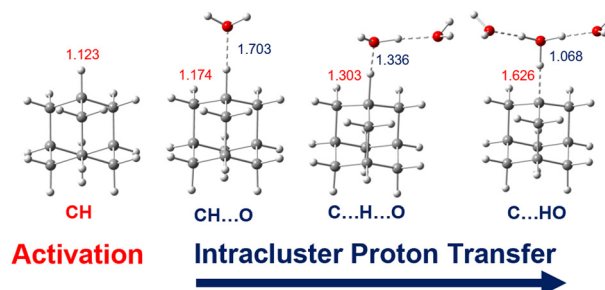


## RESEARCH PAPERS

13593

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

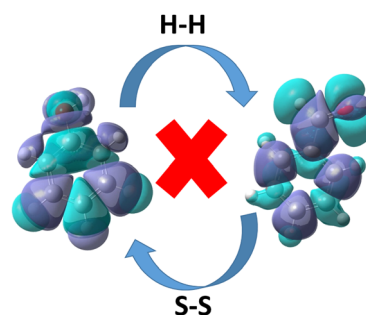
Martin Andreas Robert George and Otto Dopfer\*



13611

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

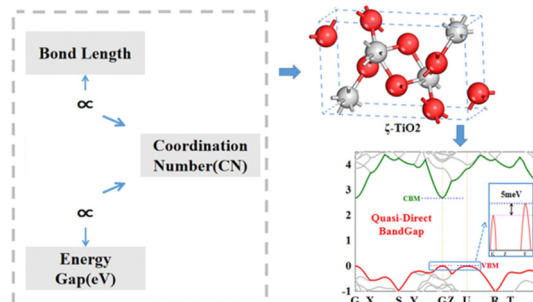
Ramón Alain Miranda-Quintana,\* Alberto Vela, Frank De Proft, Marco Martínez González and José L. Gázquez



13623

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

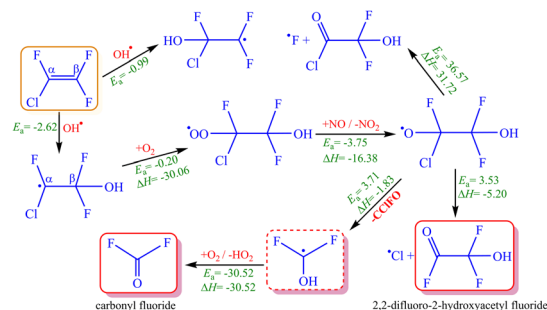
Jiayi Guo, Wangping Xu, Juexian Cao\* and Xiaolin Wei\*



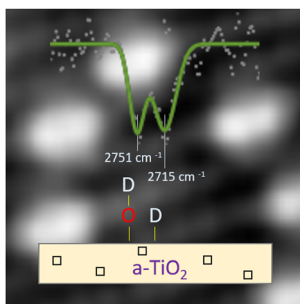
13630

### 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



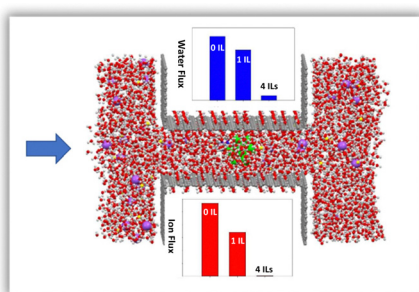
13645



### 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\*

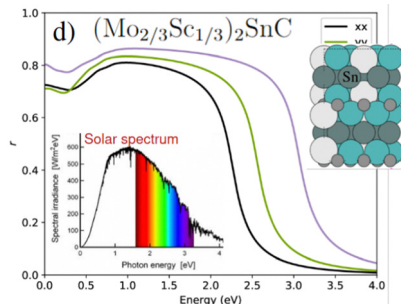
13654



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

Mohsen Abbaspour

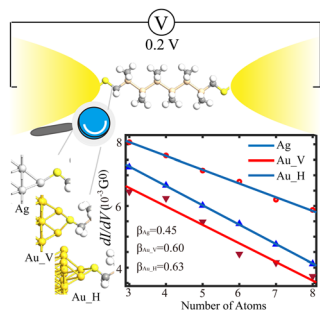
13665



### 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

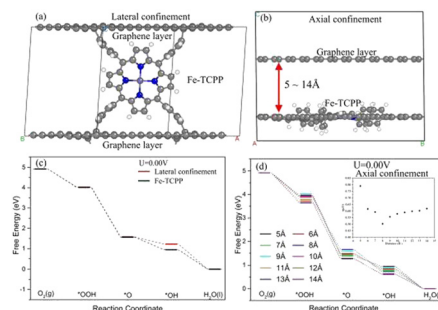
Minglang Wang,\* Xianglin Chen, Wenjun Lu, Xinyue Tian and Guang-Ping Zhang



13683

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

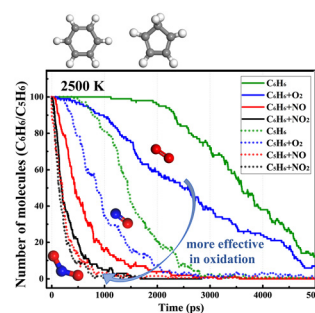
Jing-Hua Guo,\* Hong-Bo Wang, Hai-Ying Liu, Gang Chen\* and Ting-Ting Cao



13690

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

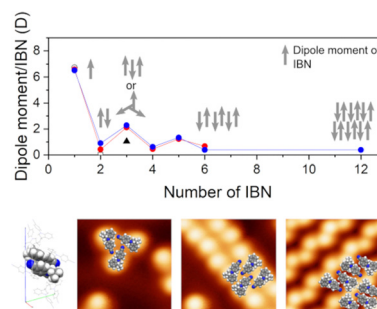
Ying Wang, Lei Zhou, Qian Mao,\* Zhanyuan Wang and Haiqiao Wei\*



13702

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

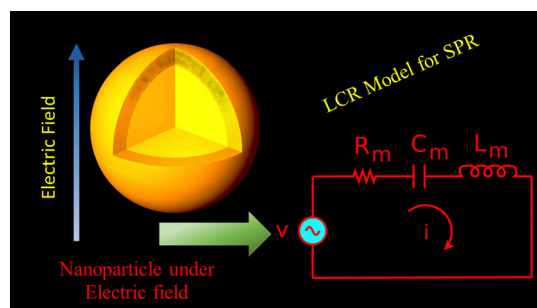
W. Nakanishi,\* Y. Matsushita, M. Takeuchi and K. Sagisaka\*



13708

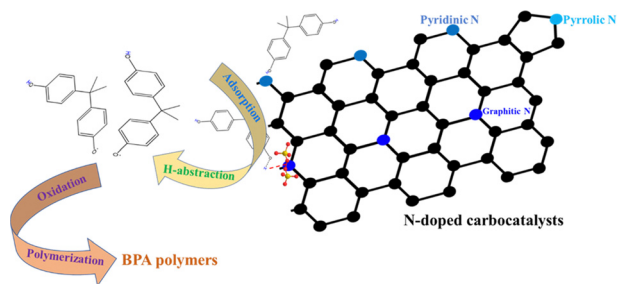
### Surface plasmon resonance in metal nanospheres explained with LCR circuits

Shivangi Dubey, Kuldeep Kumar\* and P. Arun



## RESEARCH PAPERS

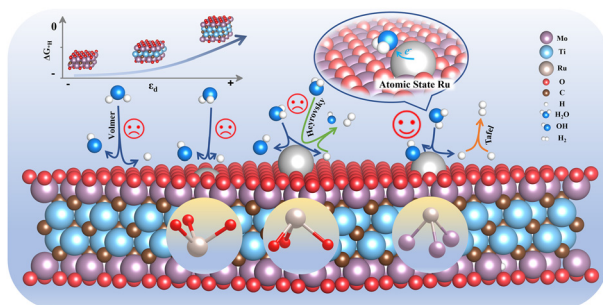
13716



### 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\*

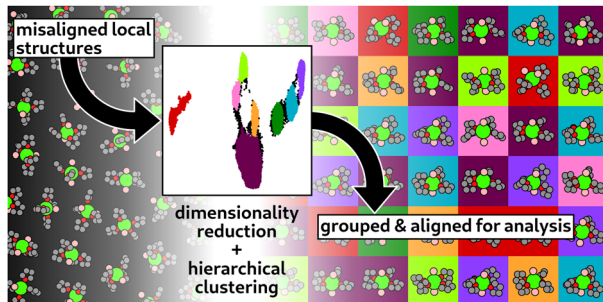
13728



### 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

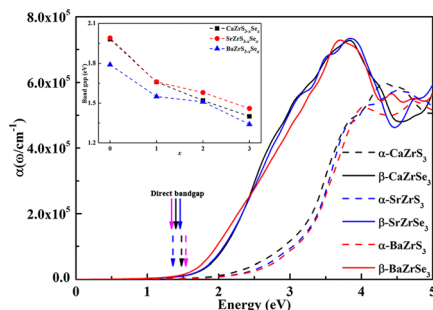
13741



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

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

13755



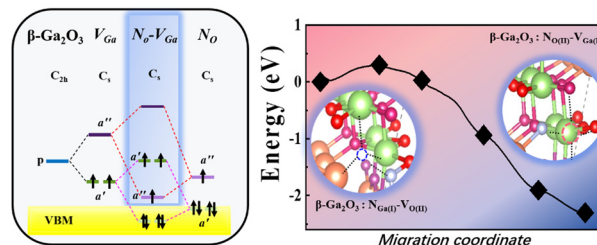
### Computational study of the fundamental properties of Zr-based chalcogenide perovskites for optoelectronics

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

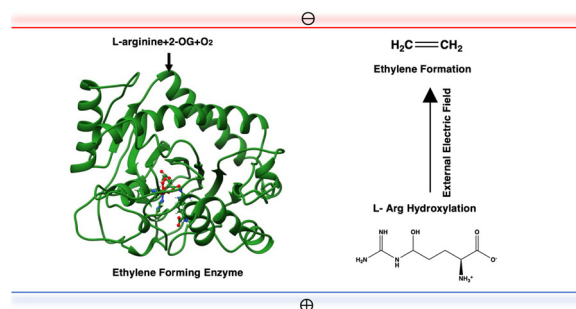


## RESEARCH PAPERS

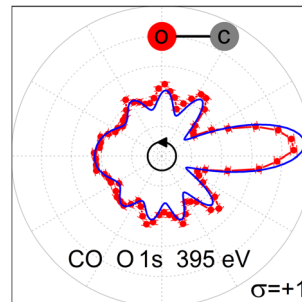
13766

**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

