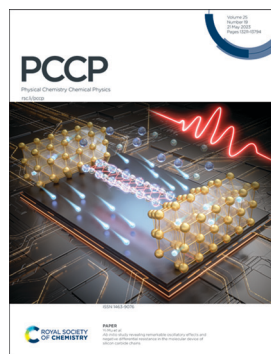


IN THIS ISSUE

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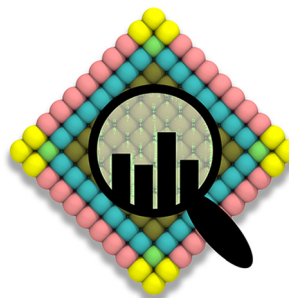
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TUTORIAL REVIEW

13228

In silico characterization of nanoparticles

Björn Kirchhoff,* Christoph Jung, Daniel Gaissmaier,
Laura Braunwarth, Donato Fantauzzi and Timo Jacob*

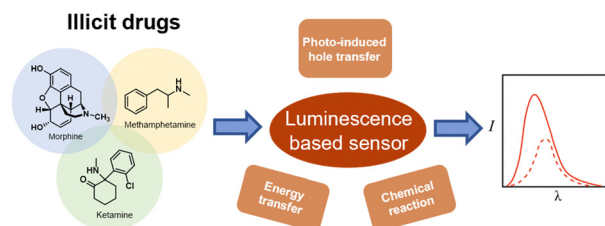


PERSPECTIVE

13244

Luminescence-based detection and identification of illicit drugs

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



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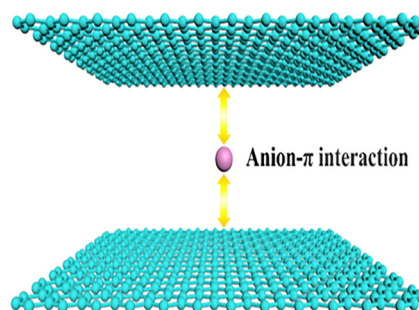


COMMUNICATION

13260

An anomalous anion transfer order in graphene oxide membranes induced by anion- π interactions

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

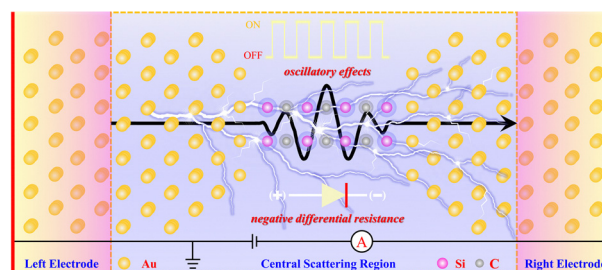


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13265

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

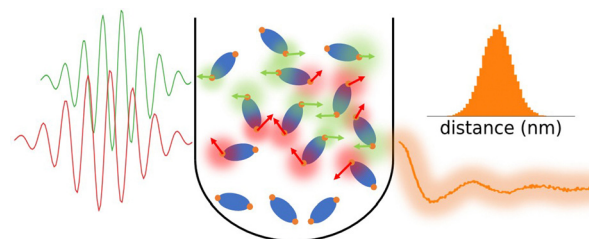
Yi Mu,* Jie Yu, Rui Hu, Cui-Hong Wang, Cai Cheng and Bang-Pin Hou



13275

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

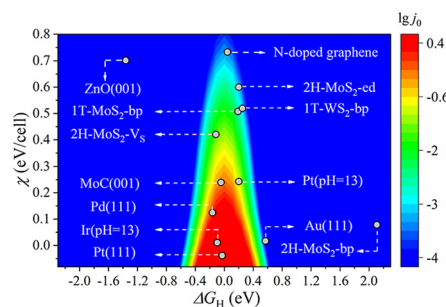
Zikri Hasanbasri, Nicholas A. Moriglioni and Sunil Saxena*



13289

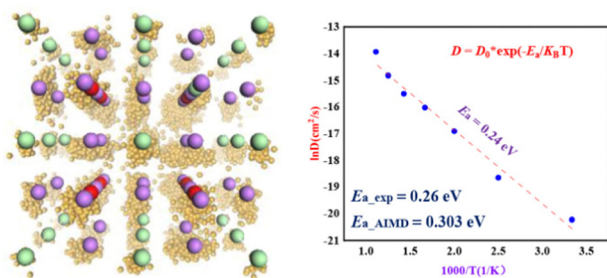
Electronegativity principle for hydrogen evolution activity using first-principles calculations

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



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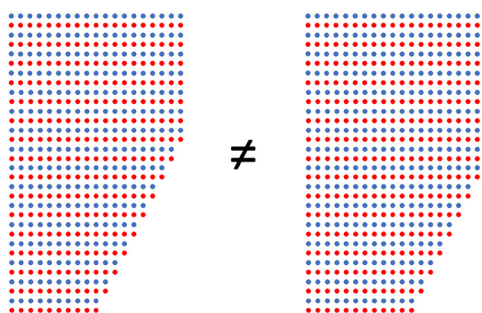
13297



Li ion diffusion behavior of Li_3OCl solid-state electrolytes with different defect structures: insights from the deep potential model

Zhou Zhang, Zhongyun Ma* and Yong Pei*

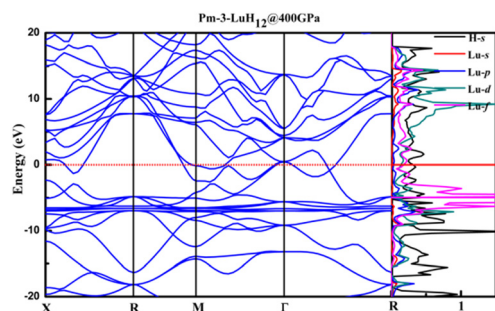
13308



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

Michael Springborg,* Meijuan Zhou and Bernard Kirtman

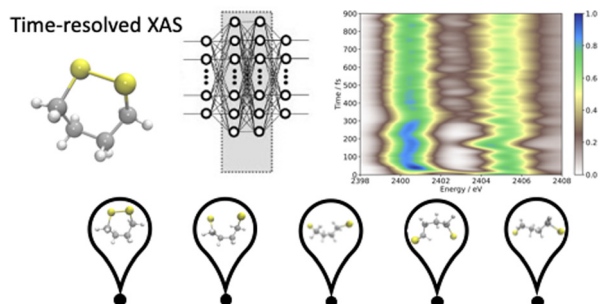
13320



Pressure-induced stability and superconductivity in LuH_{12} polyhydrides

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

13325



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*

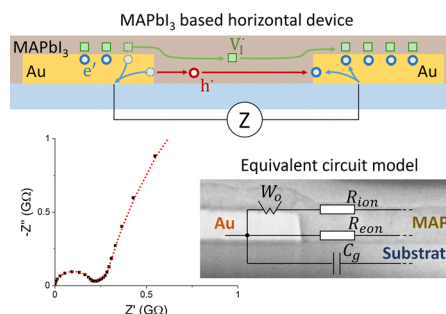


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13335

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

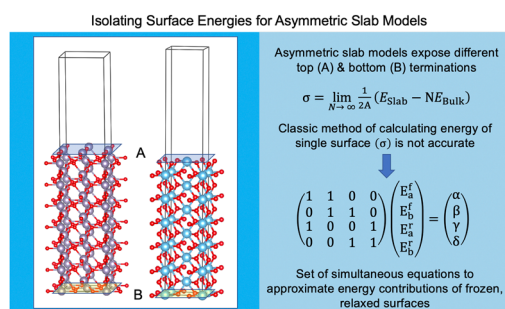
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13351

A method of calculating surface energies for asymmetric slab models

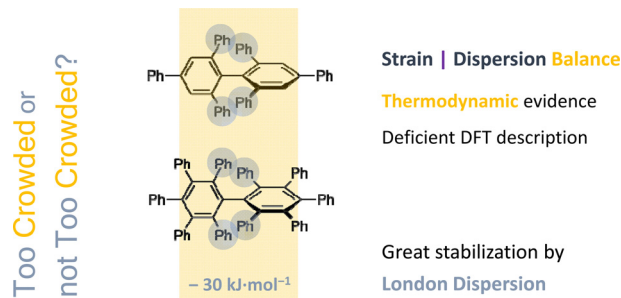
Natalie M. Stuart* and Karl Sohlberg



13359

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

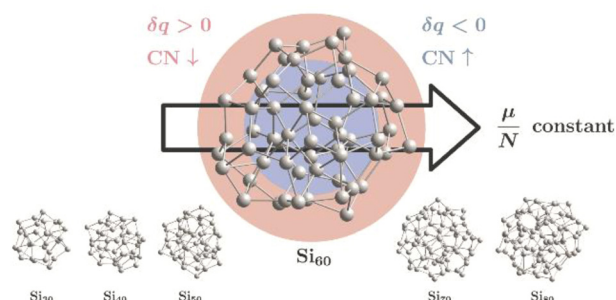
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13376

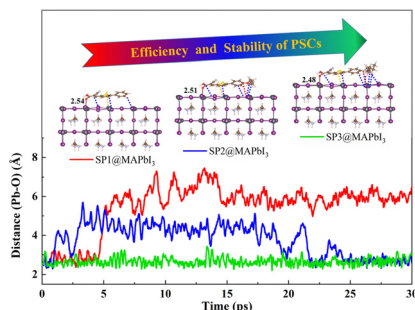
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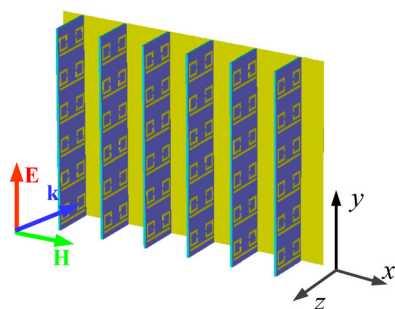
13383



Cooperative multiple interactions of donor- π -acceptor dyes enhance the efficiency and stability of perovskite solar cells

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

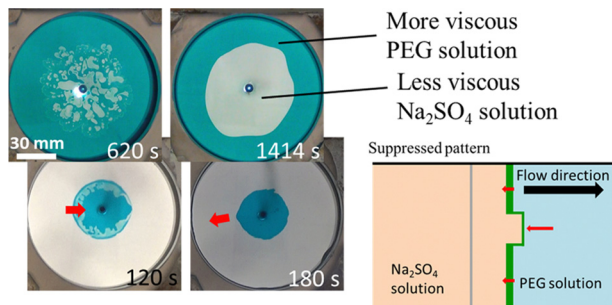
13393



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

Mingming Chen* and Xue-Xia Yang*

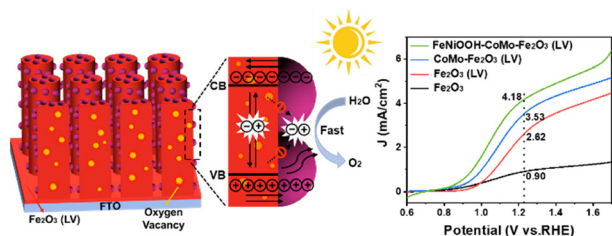
13399



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*

13410



CoMoO₄-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*

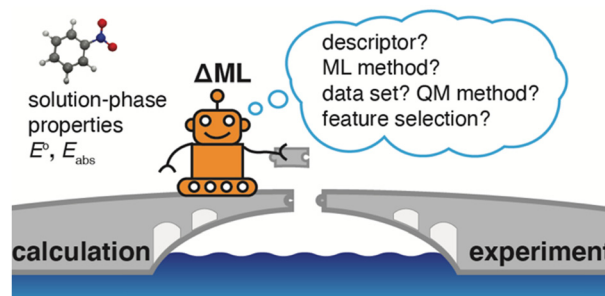


RESEARCH PAPERS

13417

Δ -Machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states

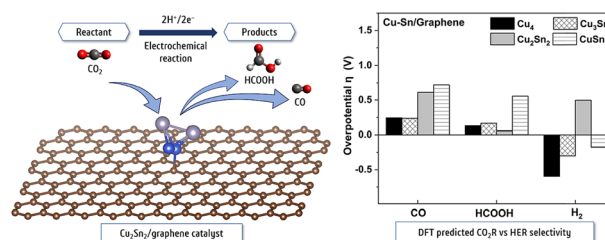
Xu Chen, Pinyuan Li, Eugen Hruska and Fang Liu*



13429

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

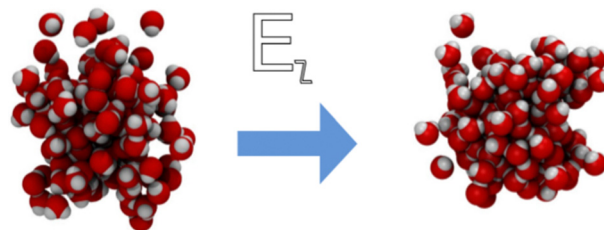
Akshayini Muthuperianayagam, Azeem Ghulam Nabi, Qi Zhao, Aman-ur-Rehman and Devis Di Tommaso*



13442

Vibrational dynamics of liquid water in an external electric field

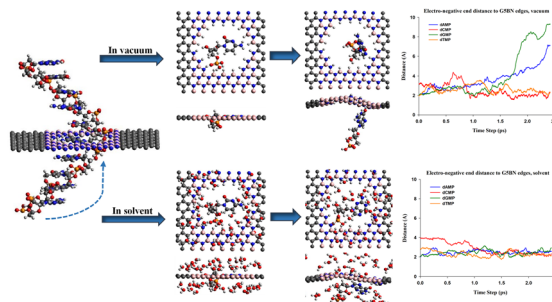
Deepak Ojha* and Thomas D. Kühne



13452

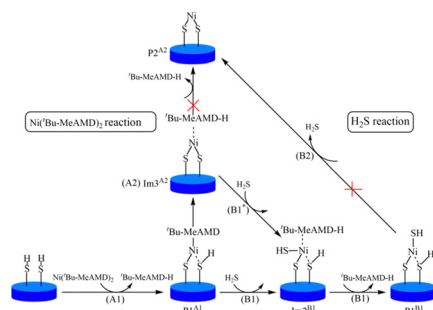
Exploring the dynamics of DNA nucleotides in graphene/h-BN nanopores: insights from *ab initio* molecular dynamics

Ali Kiakojouri, Irmgard Frank and Ebrahim Nadimi*



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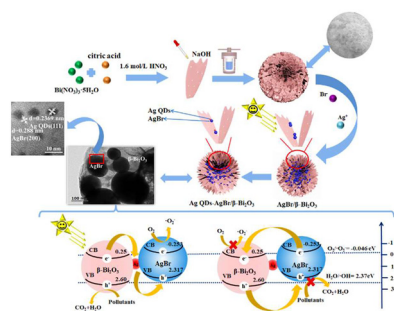
13465



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*

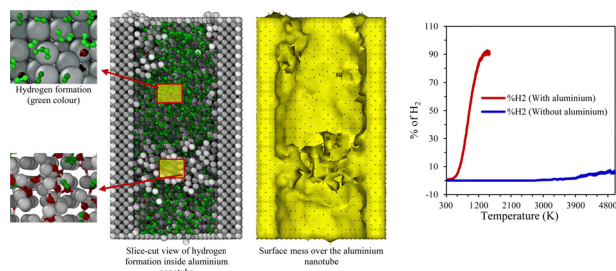
13474



Construction of a Z-scheme heterojunction bifunctional photocatalyst with Ag-modified AgBr embedded in β - Bi_2O_3 flowers

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

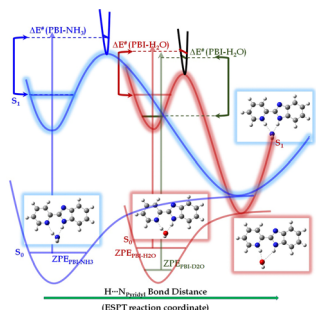
13487



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*

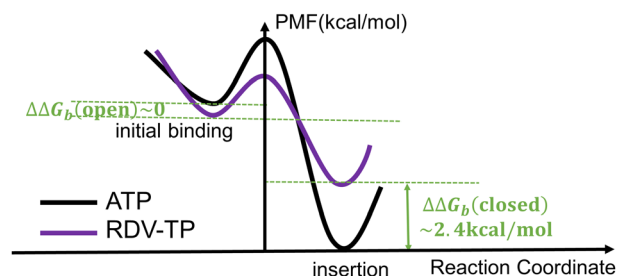


RESEARCH PAPERS

13508

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

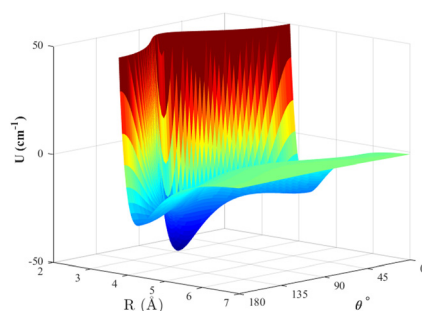
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13521

Quantum mechanical and classical calculation of the transport and relaxation properties of He...CO₂ complex using a new PES

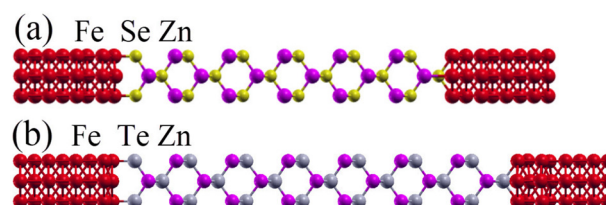
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13533

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

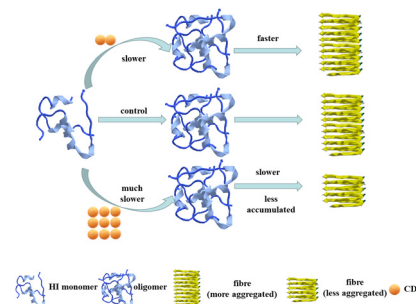
Gokaran Shukla, Hasan M. Abdullah, Avijeet Ray, Shubham Tyagi, Aurélien Manchon, Stefano Sanvito and Udo Schwingenschlögl*



13542

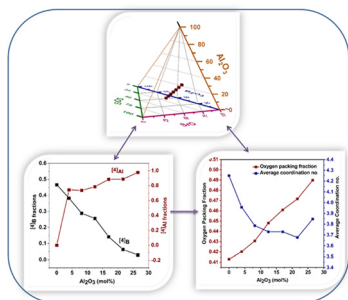
Regulation mechanism of human insulin fibrillation by L-lysine carbon dots: low concentration accelerates but high concentration inhibits the fibrillation process

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



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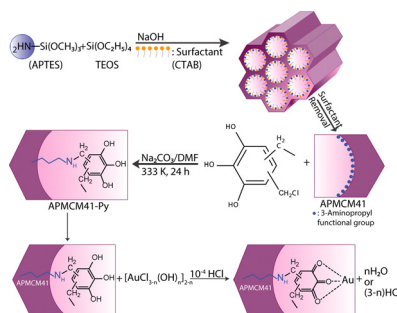
13550



An investigation of Al_2O_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*

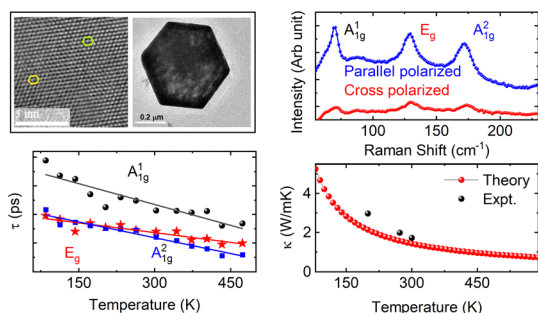
13560



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

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

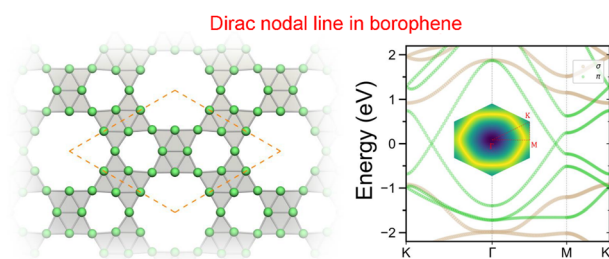
13577



Lattice thermal conductivity of topological insulator Bi_2Se_3 nanocrystals: comparison from theoretical and experimental

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

13587



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

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

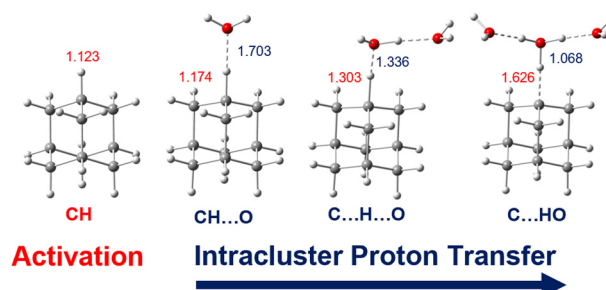


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13593

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

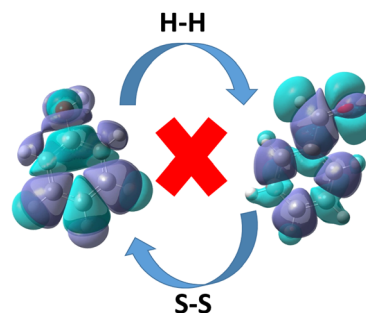
Martin Andreas Robert George and Otto Dopfer*



13611

Can we predict ambident regioselectivity using the chemical hardness?

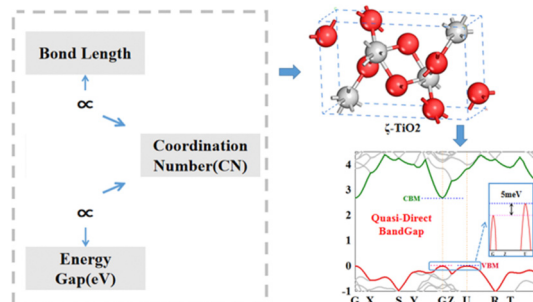
Ramón Alain Miranda-Quintana,* Alberto Vela, Frank De Proft, Marco Martínez González and José L. Gázquez



13623

Novel three-dimensional TiO_2 structure with a unique quasi-direct band gap for photocatalysts

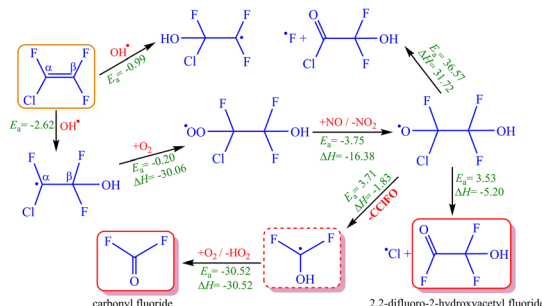
Jiayi Guo, Wangping Xu, Juexian Cao* and Xiaolin Wei*



13630

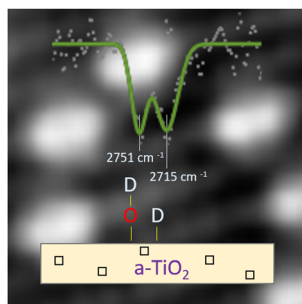
Understanding the kinetics and atmospheric degradation mechanism of chlorotrifluoroethylene ($\text{CF}_2=\text{CFCl}$) initiated by OH radicals

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



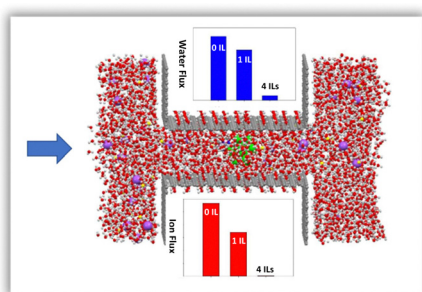
RESEARCH PAPERS

13645

**Origin of hydroxyl pair formation on reduced anatase $\text{TiO}_2(101)$**

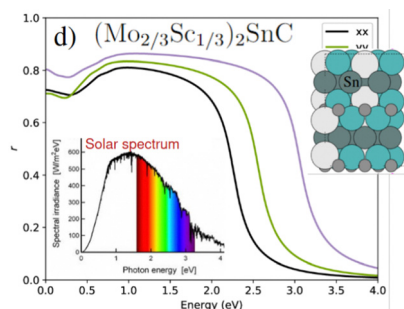
Kræn C. Adamsen, Nikolay G. Petrik,* Wilke Dononelli, Greg A. Kimmel, Tao Xu, Zheshen Li, Lutz Lammich, Bjørk Hammer, Jeppe V. Lauritsen and Stefan Wendt*

13654

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

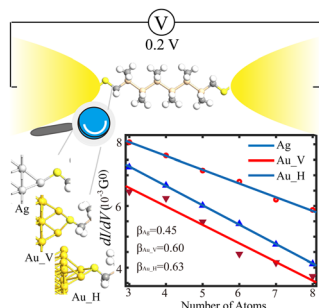
Mohsen Abbaspour

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

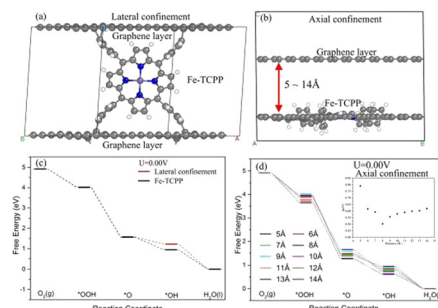


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13683

Exploration of spatial confinement and ligand effects for the oxygen reduction reaction on Fe–N_x embedded hole-graphene

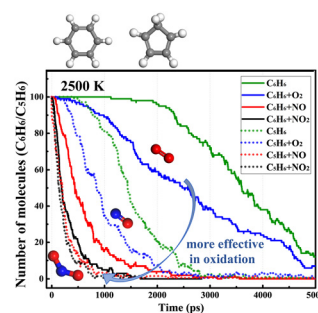
Jing-Hua Guo,* Hong-Bo Wang, Hai-Ying Liu, Gang Chen* and Ting-Ting Cao



13690

Pyrolysis and oxidation of benzene and cyclopentadiene by NO_x: a ReaxFF molecular dynamics study

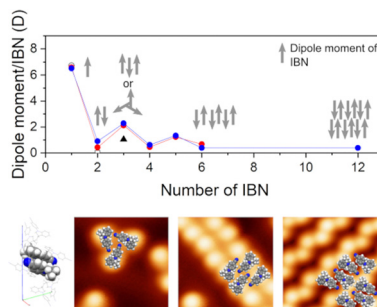
Ying Wang, Lei Zhou, Qian Mao,* Zhanyuan Wang and Haiqiao Wei*



13702

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

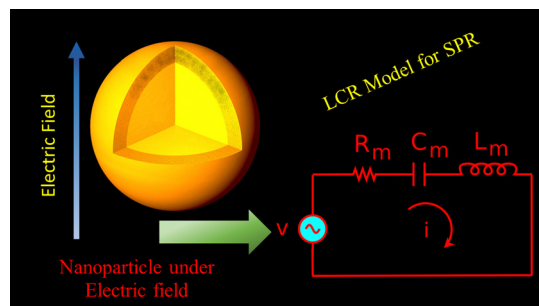
W. Nakanishi,* Y. Matsushita, M. Takeuchi and K. Sagisaka*



13708

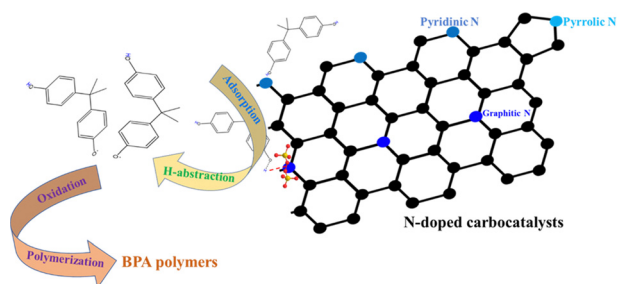
Surface plasmon resonance in metal nanospheres explained with LCR circuits

Shivangi Dubey, Kuldeep Kumar* and P. Arun



RESEARCH PAPERS

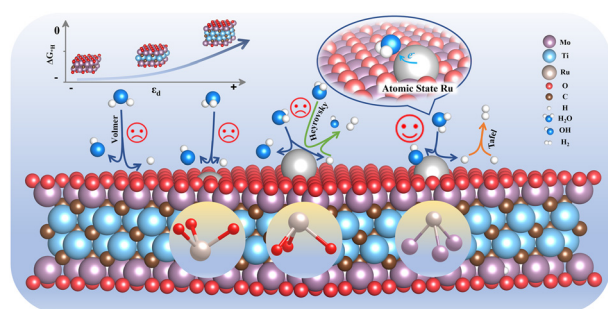
13716



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*

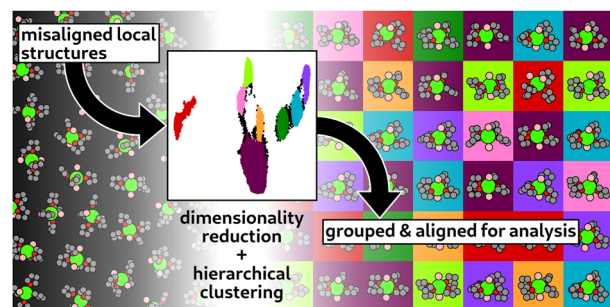
13728



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

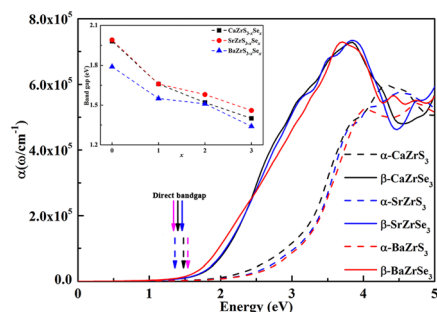
13741



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*

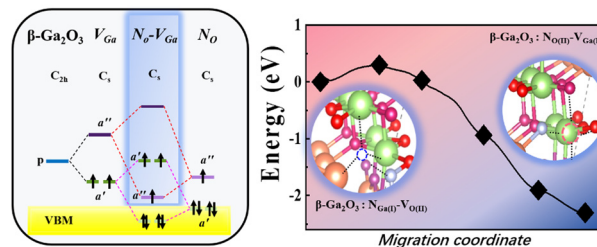


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13766

P-type nitrogen-doped β -Ga₂O₃: the role of stable shallow acceptor N_O-V_{Ga} complexes

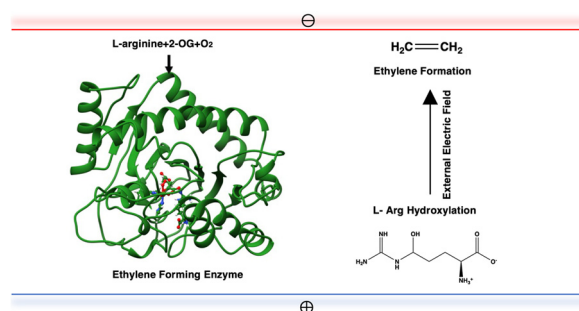
Congcong Ma, Zhengyuan Wu, Hao Zhang,*
Heyuan Zhu, Junyong Kang, Junhao Chu and Zhilai Fang*



13772

Can an external electric field switch between ethylene formation and L-arginine hydroxylation in the ethylene forming enzyme?

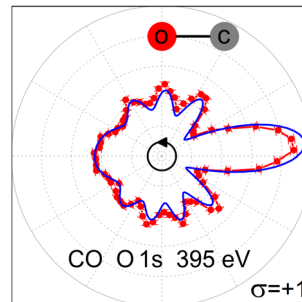
Shobhit S. Chaturvedi, Simahudeen Bathir
Jaber Sathik Rifayee, Rajeev Ramanan, Joel A. Rankin,
Jian Hu, Robert P. Hausinger and Christo Z. Christov*



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

