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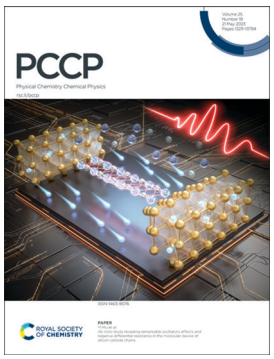

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Björn Kirchhoff,* Christoph Jung, Daniel Gaissmaier, Laura Braunwarth, Donato Fantauzzi and Timo Jacob*

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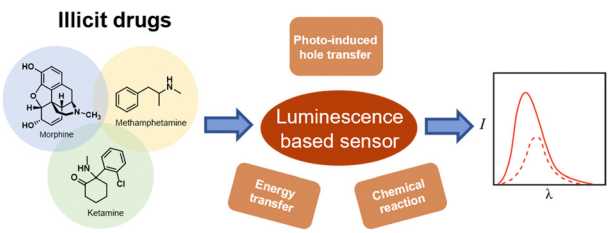
M. Chen, P. L. Burn* and P. E. Shaw*



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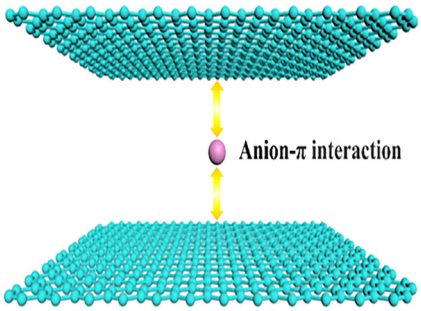
COMMUNICATION

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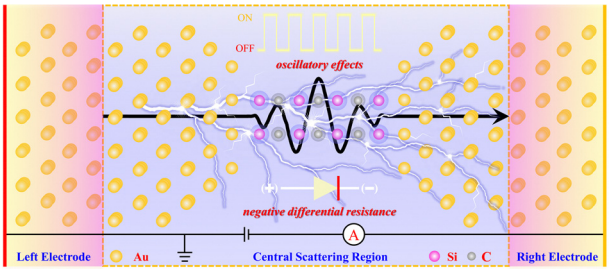
***Ab initio* study revealing remarkable oscillatory effects and negative differential resistance in the molecular device of silicon carbide chains**

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



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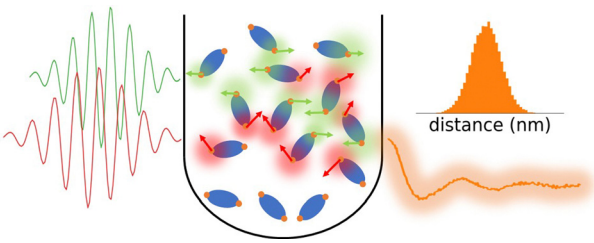
Efficient sampling of molecular orientations for Cu(II)-based DEER on protein labels

Zikri Hasanbasri, Nicholas A. Moriglioni and Sunil Saxena*



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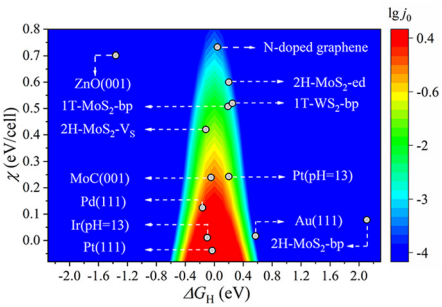
Electronegativity principle for hydrogen evolution activity using first-principles calculations

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



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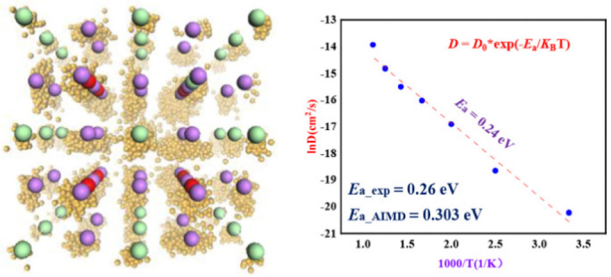

Li ion diffusion behavior of Li_3OCl solid-state electrolytes with different defect structures: insights from the deep potential model

Zhou Zhang, Zhongyun Ma* and Yong Pei*

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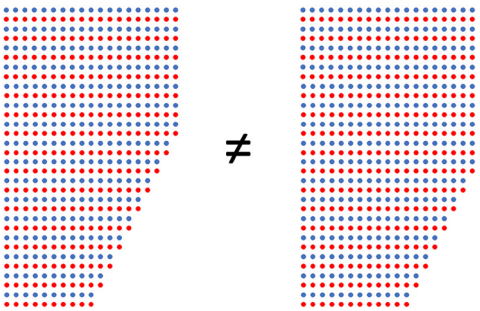

The shape effect and its consequences for polar surfaces and for heterogeneous catalysis

Michael Springborg,* Meijuan Zhou and Bernard Kirtman

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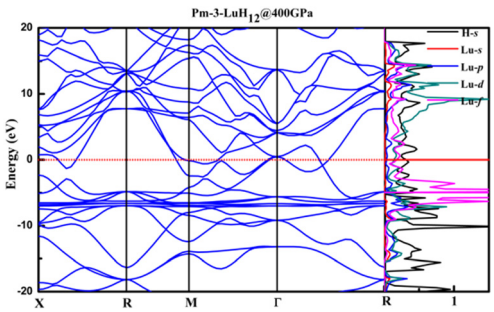

Pressure-induced stability and superconductivity in LuH_{12} polyhydrides

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

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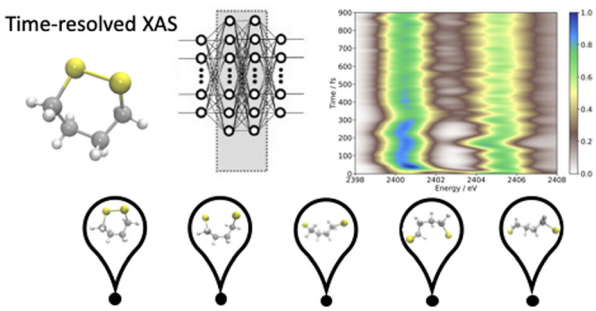

An on-the-fly deep neural network for simulating time-resolved spectroscopy: predicting the ultrafast ring opening dynamics of 1,2-dithiane

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

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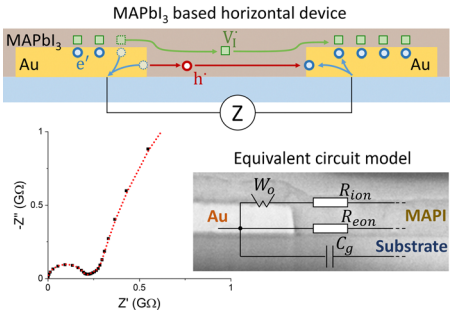
Ionic and electronic polarization effects in horizontal hybrid perovskite device structures close to equilibrium

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



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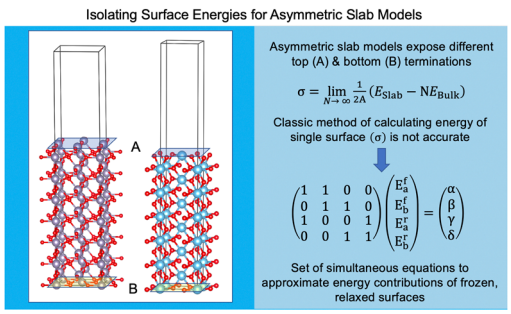
A method of calculating surface energies for asymmetric slab models

Natalie M. Stuart* and Karl Sohlberg



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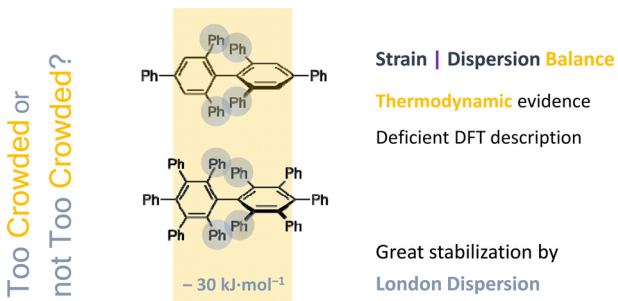
How great is the stabilization of crowded polyphenylbiphenyls by London dispersion?

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



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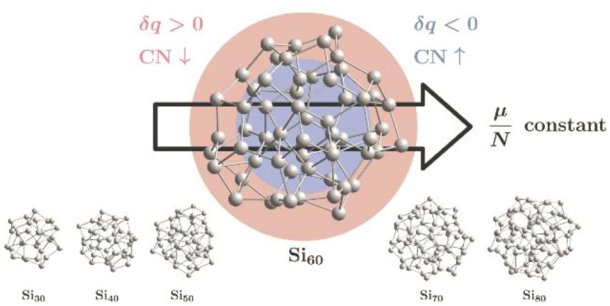
Scaling of the permanent electric dipole moment in isolated silicon clusters with near-spherical shape

Filip Rivic,* Andreas Lehr and Rolf Schäfer



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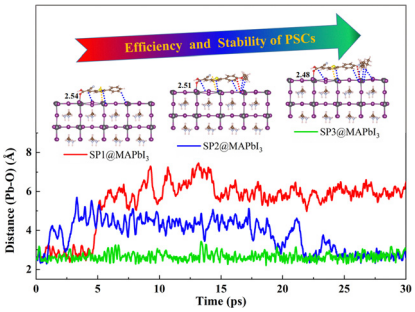

Cooperative multiple interactions of donor–π–acceptor dyes enhance the efficiency and stability of perovskite solar cells

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

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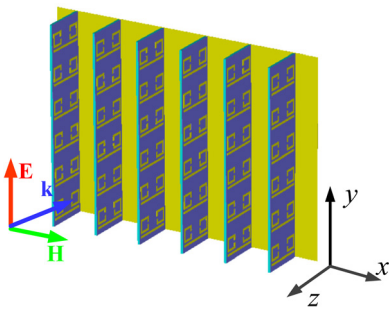

Tunable and three-dimensional dual-band metamaterial absorber based on electromagnetically induced transparency with vanadium dioxide

Mingming Chen* and Xue-Xia Yang*

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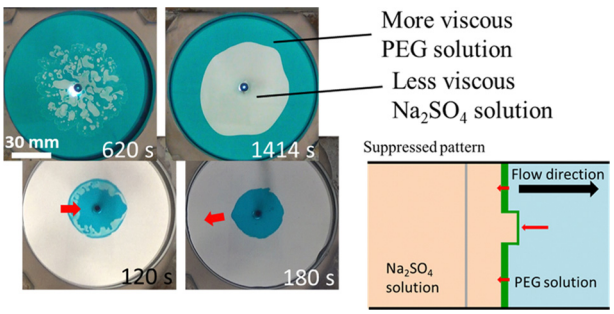

Experimental demonstration of the suppression of viscous fingering in a partially miscible system

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

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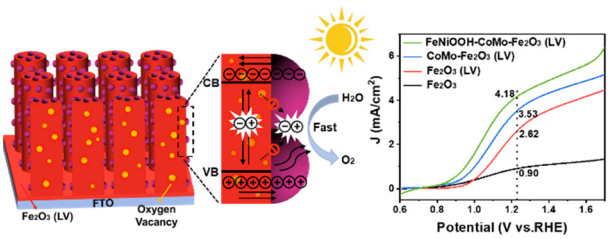

$CoMoO_4$-modified hematite with oxygen vacancies for high-efficiency solar water splitting

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

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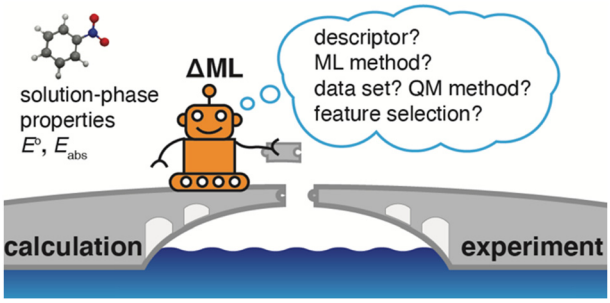
Δ-Machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states

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



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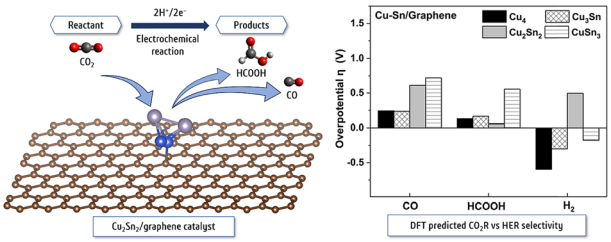
Adsorption, activation, and conversion of carbon dioxide on small copper–tin nanoclusters

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



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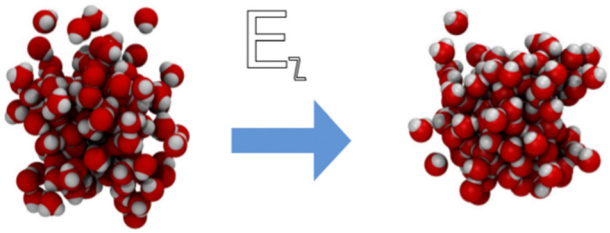
Vibrational dynamics of liquid water in an external electric field

Deepak Ojha* and Thomas D. Kühne



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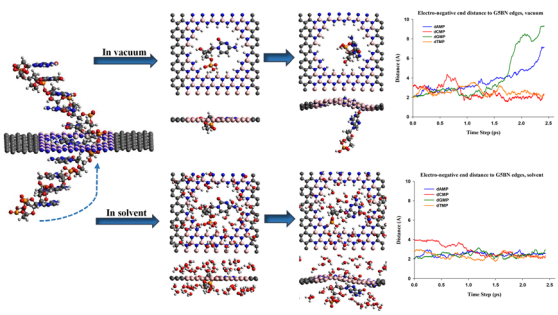
Exploring the dynamics of DNA nucleotides in graphene/h-BN nanopores: insights from *ab initio* molecular dynamics

Ali Kiakojouri, Irmgard Frank and Ebrahim Nadimi*



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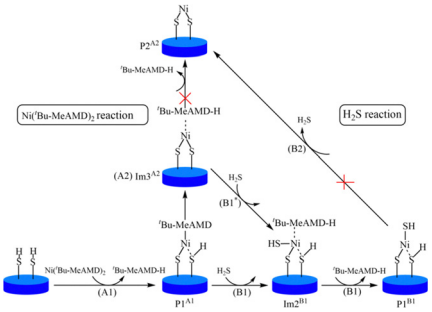

Reaction mechanism of nickel sulfide atomic layer deposition using bis(*N*,*N*′-di-*tert*-butylacetamidinato)nickel(II) and hydrogen sulfide

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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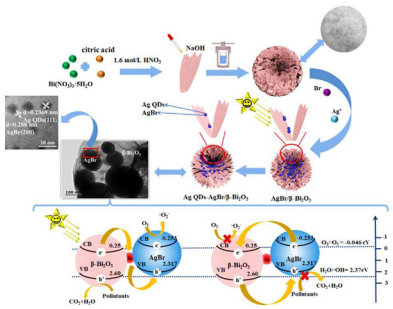

Construction of a Z-scheme heterojunction bifunctional photocatalyst with Ag-modified AgBr embedded in β-Bi_2O_3 flowers

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

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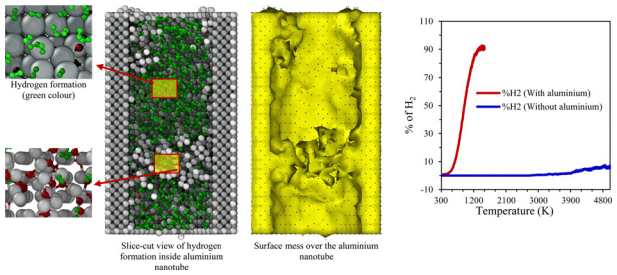
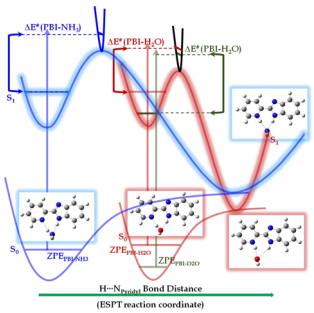


Aluminum nanotubes as an efficient catalyst for hydrogen production *via* thermochemical water splitting: a reactive molecular dynamics simulation

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*

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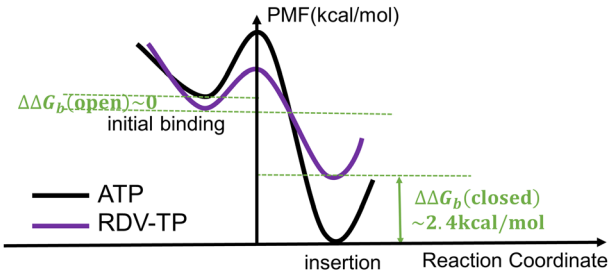
13508

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

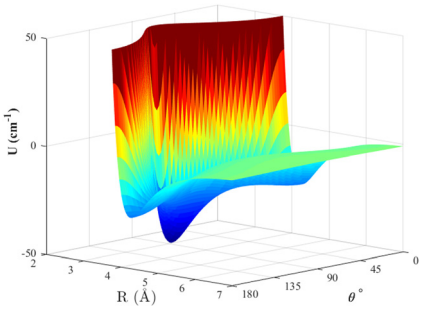
Chunhong Long, Moises Ernesto Romero, Liqiang Dai and Jin Yu*



13521

Quantum mechanical and classical calculation of the transport and relaxation properties of He···CO_2 complex using a new PES

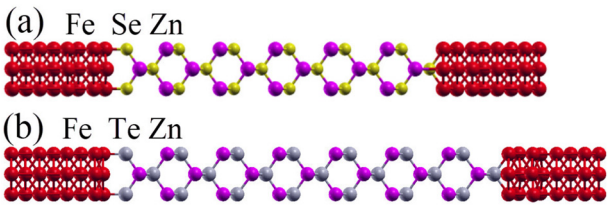
Ebrahim Nemati-Kande,* Fatemeh Aghababaei and Salar Sadeghi



13533

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

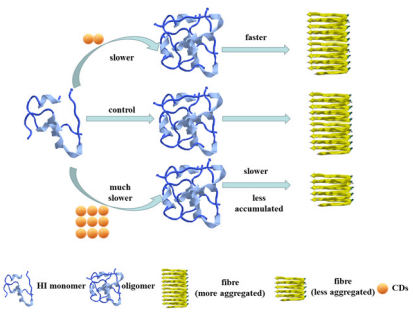
Gokaran Shukla, Hasan M. Abdullah, Avijeet Ray, Shubham Tyagi, Aurélien Manchon, Stefano Sanvito and Udo Schwingenschlögl*



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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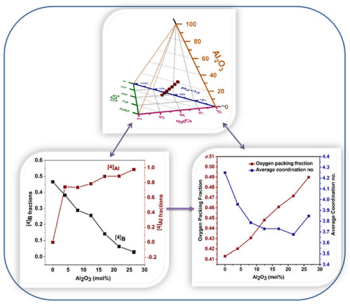
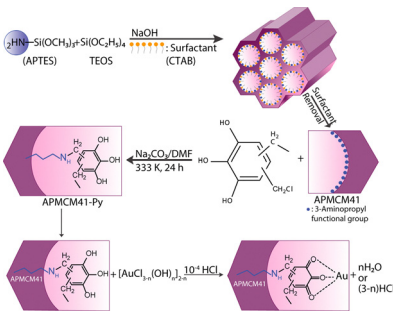
13550



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*

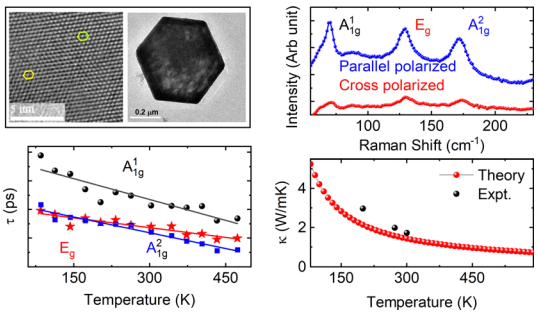
13560



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

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

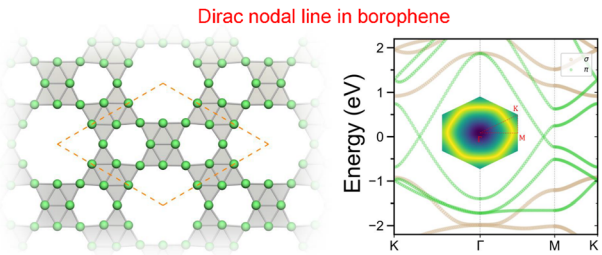
13577



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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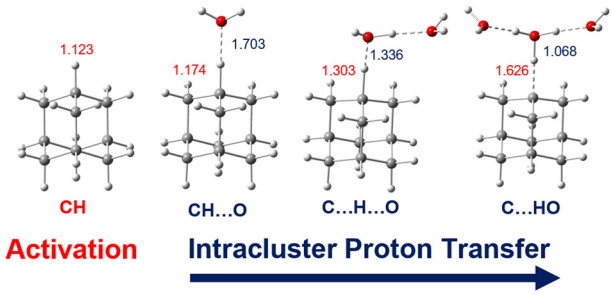
13593

Microhydration of the adamantane cation: intracluster proton transfer to solvent in $[Ad(H_2O)_{n=1-5}]^+$ for $n \geq 3$

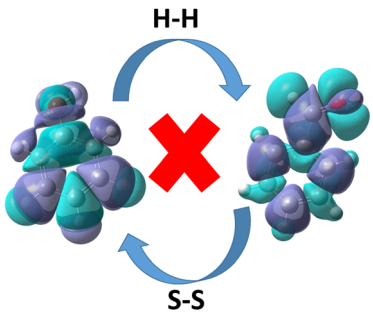
Martin Andreas Robert George and Otto Dopfer*



13611

Can we predict ambident regioselectivity using the chemical hardness?

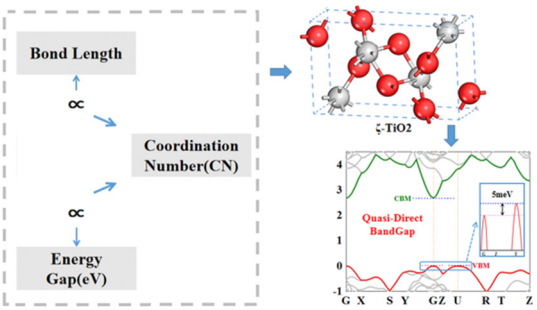
Ramón Alain Miranda-Quintana,* Alberto Vela, Frank De Proft, Marco Martínez González and José L. Gázquez



13623

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

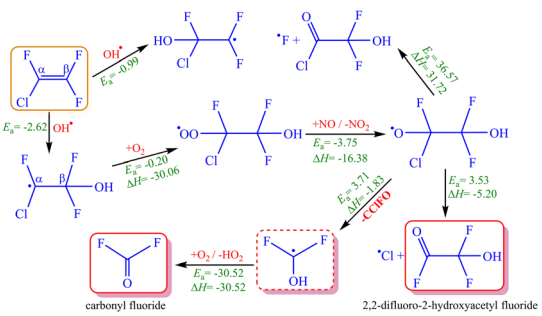
Jiayi Guo, Wangping Xu, Juexian Cao* and Xiaolin Wei*



13630

Understanding the kinetics and atmospheric degradation mechanism of chlorotrifluoroethylene (CF_2═CFCl) initiated by OH radicals

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



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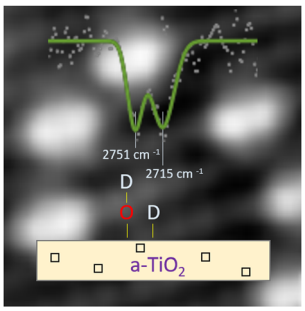
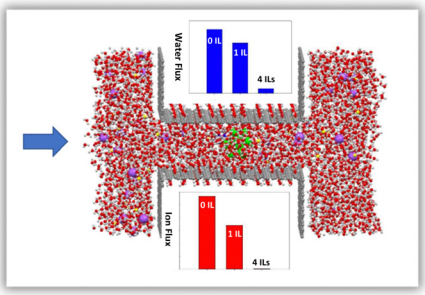
13645



Origin of hydroxyl pair formation on reduced anatase 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*

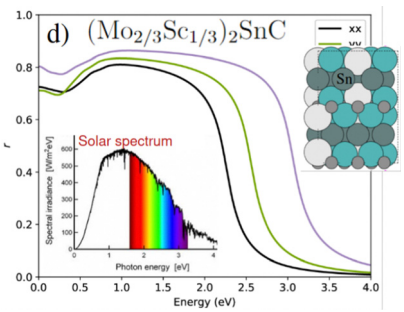
13654



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

Mohsen Abbaspour

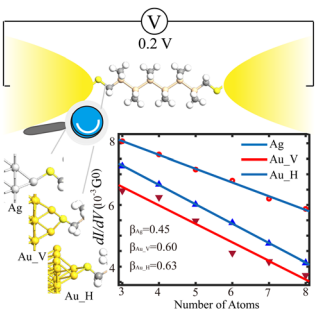
13665



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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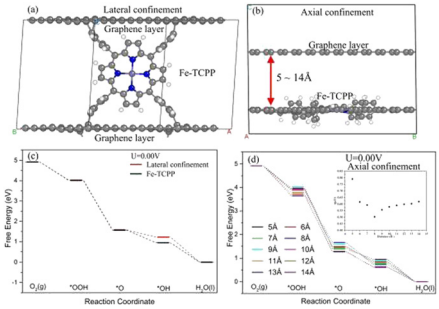
13683

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

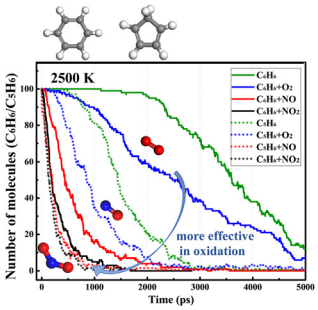
Jing-Hua Guo,* Hong-Bo Wang, Hai-Ying Liu, Gang Chen* and Ting-Ting Cao



13690

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

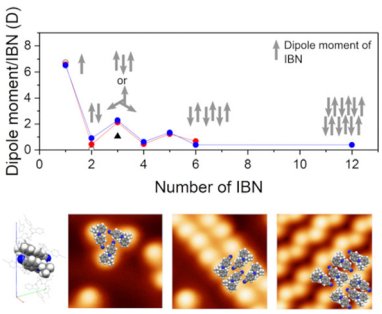
Ying Wang, Lei Zhou, Qian Mao,* Zhanyuan Wang and Haiqiao Wei*



13702

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

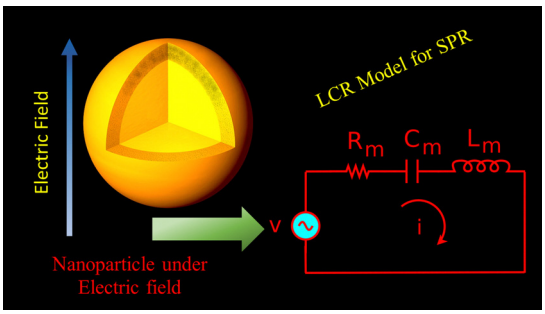
W. Nakanishi,* Y. Matsushita, M. Takeuchi and K. Sagisaka*



13708

Surface plasmon resonance in metal nanospheres explained with LCR circuits

Shivangi Dubey, Kuldeep Kumar* and P. Arun



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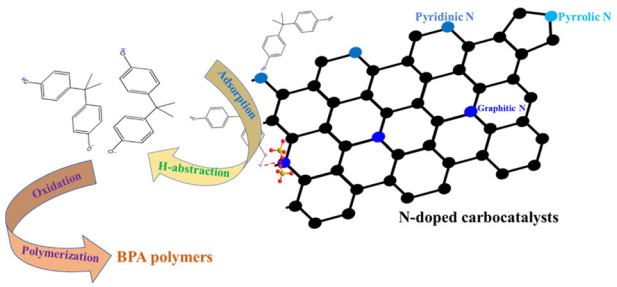
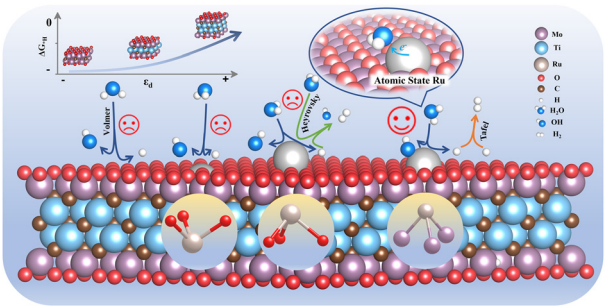
13716



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*

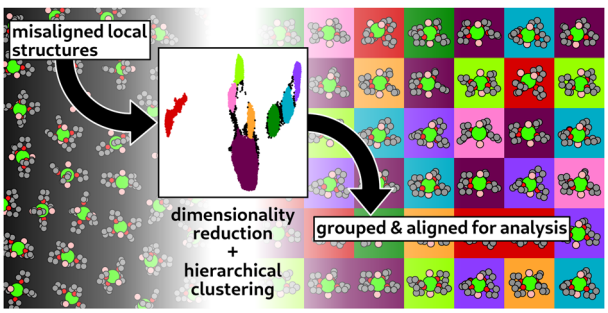
13728



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

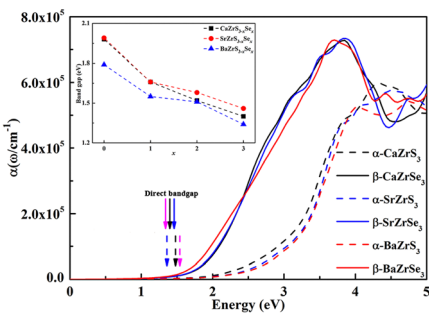
13741



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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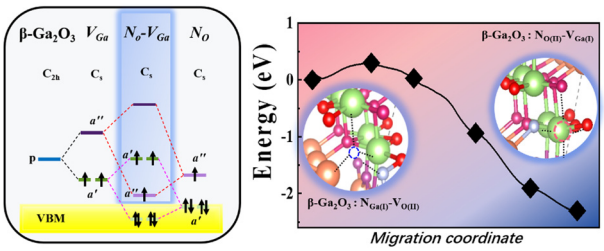
13766

P-type nitrogen-doped β-Ga_2O_3: the role of stable shallow acceptor N_O–V_{Ga} complexes

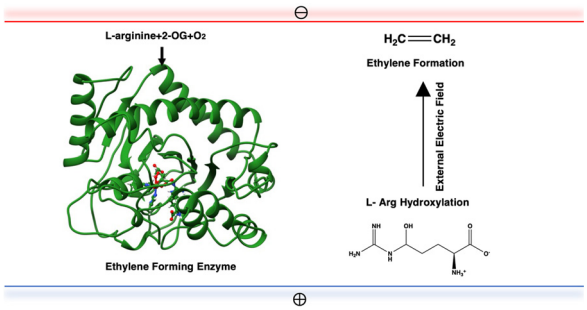
Congcong Ma, Zhengyuan Wu, Hao Zhang,*
Heyuan Zhu, Junyong Kang, Junhao Chu and Zhilai Fang*



13772

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

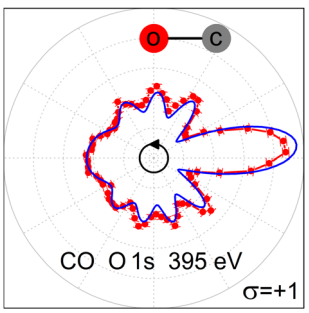
Shobhit S. Chaturvedi, Simahudeen Bathir
Jaber Sathik Rifayee, Rajeev Ramanan, Joel A. Rankin,
Jian Hu, Robert P. Hausinger and Christo Z. Christov*



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