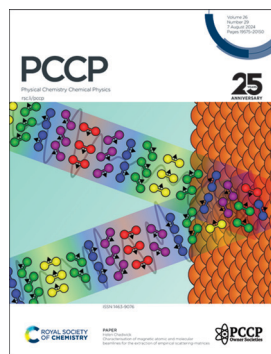


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ISSN 1463–9076 CODEN PPCPFQ 26(29) 19575–20150 (2024)



Cover

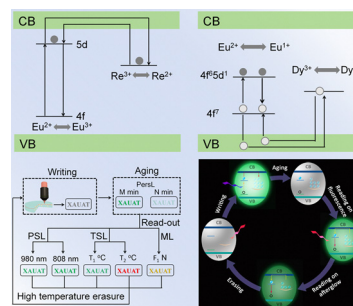
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REVIEWS

19591

Deep-trap persistent materials for future rewriteable optical information storage

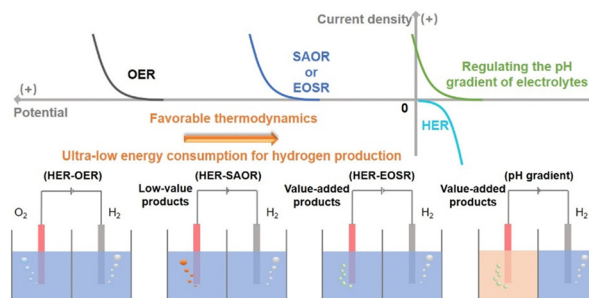
Chaoyang Jia, Jia Yu, YuanYuan Hu,
Xiaojun Wang* and Dangli Gao*



19606

Recent progress in energy-saving electrocatalytic hydrogen production via regulating the anodic oxidation reaction

Taotao Gao, Qi An, Xiangmin Tang, Qu Yue, Yang Zhang,
Bing Li, Panpan Li and Zhaoyu Jin*



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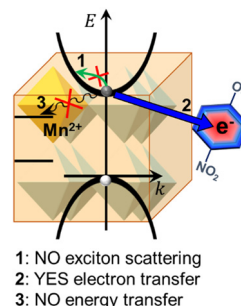


COMMUNICATION

19625

Ultrafast electron shuttling suppresses the energy transfer process in Mn-doped CsPbCl₃ nanocrystals

Tushar Debnath

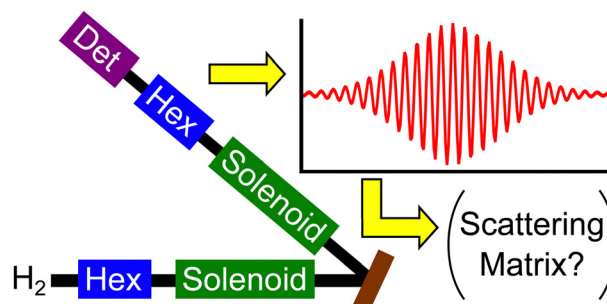


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19630

Characterisation of magnetic atomic and molecular beamlines for the extraction of empirical scattering-matrices

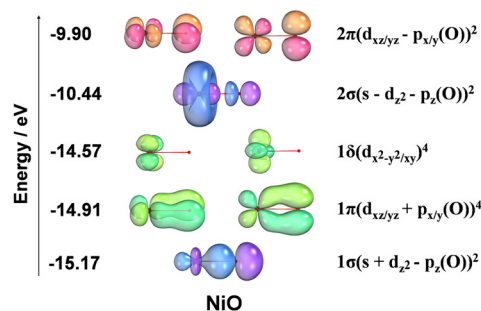
Helen Chadwick



19646

The electronic structure of diatomic nickel oxide

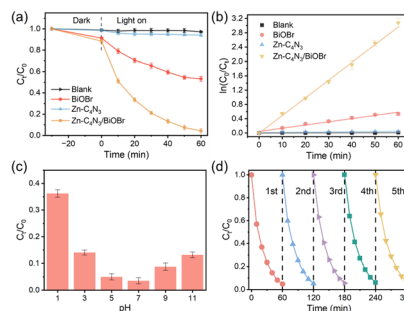
Nickolas A. Joyner, João Gabriel Farias Romeu, Brian Kent and David A. Dixon*



19658

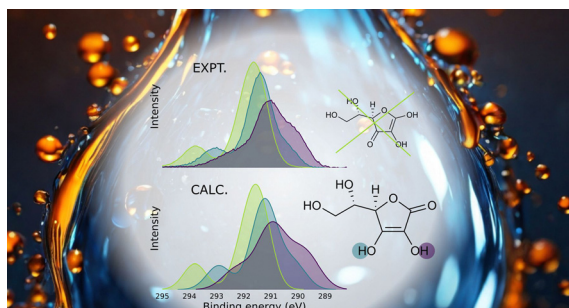
Zinc-doped C₄N₃/BiOBr S-scheme heterostructured hollow spheres for efficient photocatalytic degradation of tetracycline

Yaqi Liu, Guicheng Luo, Yichen Liu, Zuozheng Xu, Hengxin Shen, Yuxiang Sheng, Yuan Zhu, Shuyi Wu,* Lizhe Liu* and Yun Shan*



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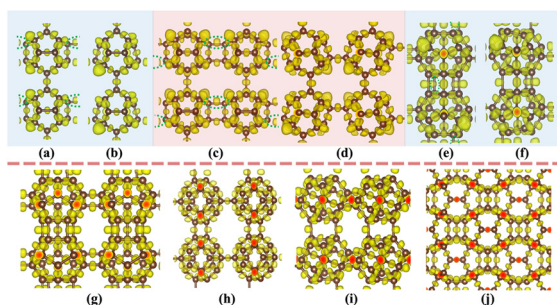
19673



Liquid-jet photoemission spectroscopy as a structural tool: site-specific acid–base chemistry of vitamin C

Lukáš Tomaník, Michele Pugini, Karen Mudryk, Stephan Thürmer, Dominik Stemer, Bruno Credidio, Florian Trinter, Bernd Winter* and Petr Slaviček*

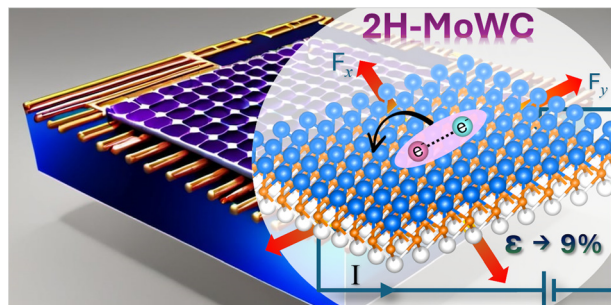
19685



Prediction of pure carbon crystals with intrinsic antiferromagnetism: polymerized from C₂₀ fullerenes

Haiping Wu,* Xinqi Hang, Erjun Kan and Yan Qian*

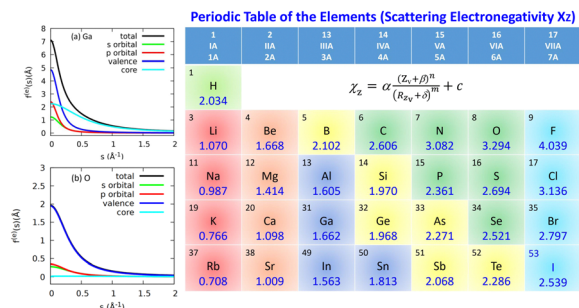
19696



First-principles study on structural stabilities, mechanical properties, and biaxial strain-induced superconductivity in Janus MoWC monolayer

Sirinee Thasitha, Prutthipong Tsuppayakorn-aek, Anan Udomkijmongkol, Satchakorn Khammuang, Thanayut Kaewmaraya, Tanveer Hussain, Thiti Bovornratanaraks and Komsilp Kotmool*

19705



Universal scales of electronegativity and ionicity from electron scattering factors

Jin-Cheng Zheng

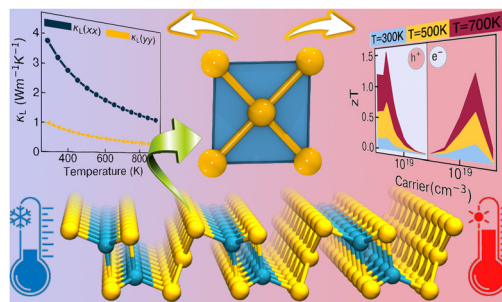


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19724

Polytelluride square planar chain-induced anharmonicity results in ultralow thermal conductivity and high thermoelectric efficiency in Al_2Te_5 monolayers

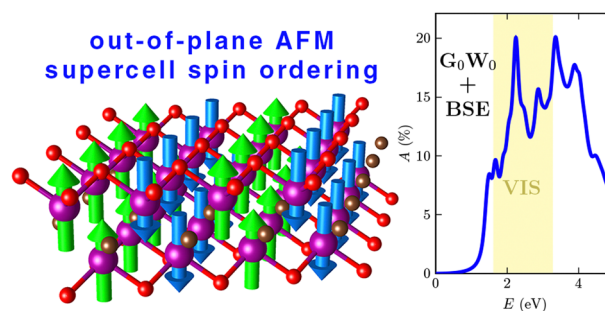
Iraj Maleki, S. Mehdi Vaez Allaei* and S. Shahab Naghavi*



19733

Mn_2C MXene functionalized by oxygen is a semiconducting antiferromagnet and an efficient visible light absorber

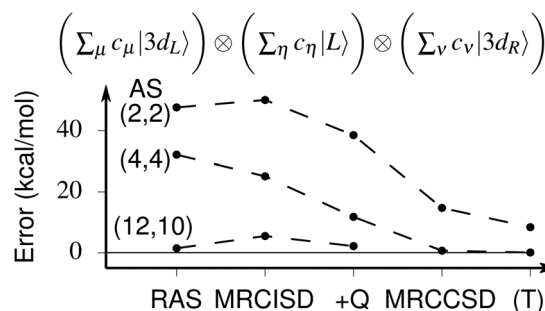
Jiří Kalmár and František Karlický*



19742

Towards reliable and efficient modeling of $[\text{Cu}_2\text{O}_2]^{2+}$ -based compound electronic structures with the partially fixed reference space protocols

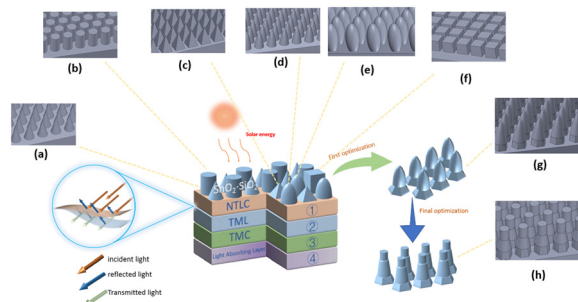
Matheus Morato F. de Moraes* and Paweł Tecmer*



19755

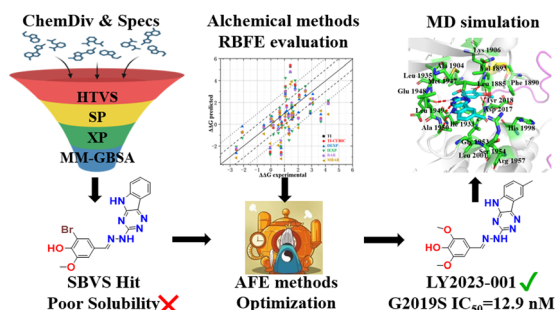
Modeling and admittance recursive simulation of anti-reflective coatings for photothermal conversion: synergy between subwavelength structures and gradient refractive index layers

Zihao Zhu, Yanyan Bu* and Xiangfu Wang*



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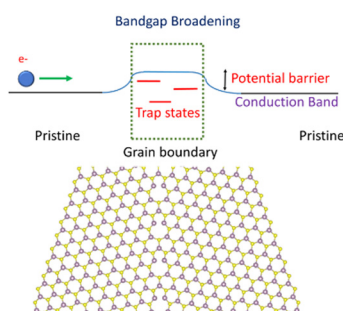
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Identification of novel LRRK2 inhibitors by structure-based virtual screening and alchemical free energy calculation

Shuoyan Tan, Xiaoqing Gong, Huanxiang Liu* and Xiaojun Yao*

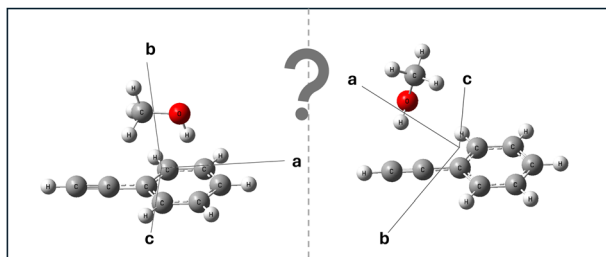
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Defect structure–electronic property correlations in transition metal dichalcogenide grain boundaries

Srest Somay and Krishna Balasubramanian*

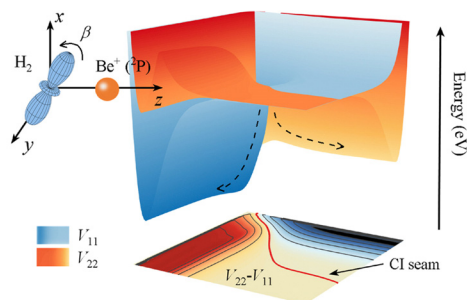
19795



Microwave spectroscopic and computational analyses of the phenylacetylene...methanol complex: insights into intermolecular interactions

Surabhi Gupta, Charlotte N. Cummings, Nicholas R. Walker and Elangannan Arunan*

19812



Stereodynamic control of nonadiabatic processes in low-energy $Be^+ (^2P) + H_2$ ($v = 0, j = 2$) collisions

Ye Mao, Hanghang Chen, Zijiang Yang, Bayaer Buren* and Maodu Chen*

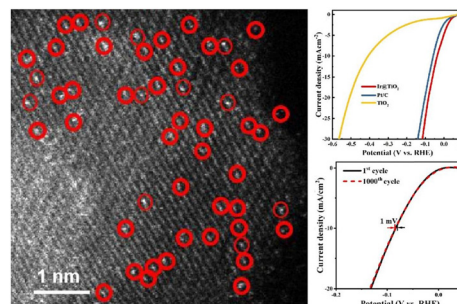


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Iridium single-atoms anchored on a TiO₂ support as an efficient catalyst for the hydrogen evolution reaction

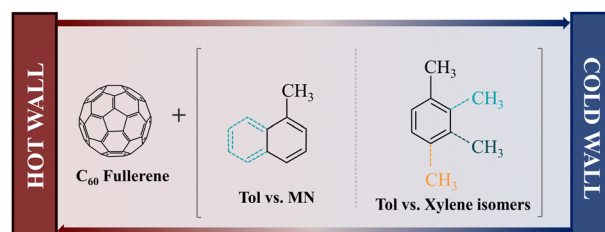
Wenxuan Li, Dashu Yin, Peng Li, Xinhua Zhao* and Shengcai Hao*



19831

Isothermal and non-isothermal transport properties of diluted fullerene binary and ternary aromatic solvent mixtures

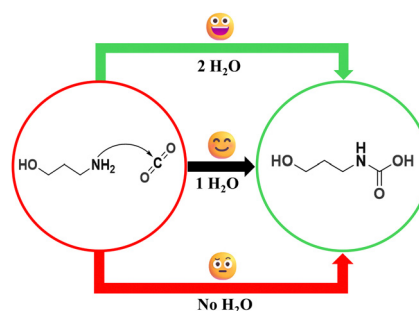
A. Errarte, D. Sommermann, V. Shevtsova, W. Köhler and M. M. Bou-Ali*



19845

Water-assisted absorption of CO₂ by 3-amino-1-propanol: a mechanistic insight

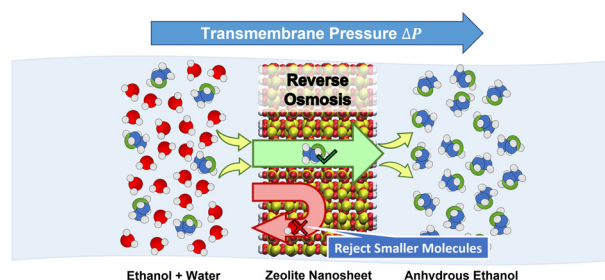
Shivam Rawat and C. N. Ramachandran*



19854

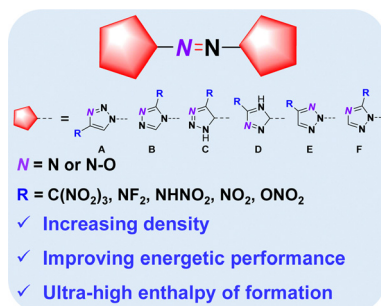
Adsorption-driven reverse osmosis separation of ethanol/water using zeolite nanosheets

Yen-Yung Wu and Li-Chiang Lin*



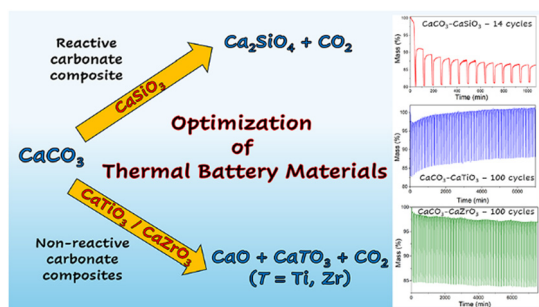
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19863

Enhancing the detonation performance of azobistriazole energetic derivatives *via* inducing *N*-oxide groups

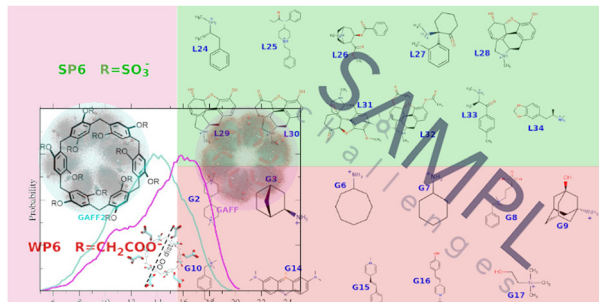
Nan Li,* Xinbo Yang, Xiuyuan Li, Zihuan Peng, Zehong Yin, Chongwen Jiang, Zhihong Huang and Yuchuan Li*

19876

Optimising thermochemical energy storage: a comprehensive analysis of $CaCO_3$ composites with $CaSiO_3$, $CaTiO_3$, and $CaZrO_3$

Terry D. Humphries,* Adriana P. Vieira, Yurong Liu, Eleanor McCabe, Mark Paskevicius and Craig E. Buckley

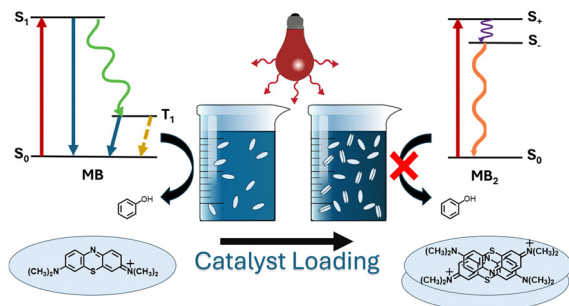
19887



Methodological and force field effects in the molecular dynamics-based prediction of binding free energies of host-guest systems

Zhaoxi Sun and Piero Procacci*

19900



Concentration-dependent aggregation of methylene blue acting as a photoredox catalyst

Benjamin J. Thompson, Anshu Kumar and Vanessa M. Huxter*

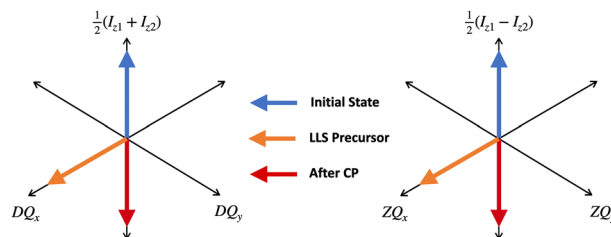


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19908

Excitation of long-lived nuclear spin order using spin-locking: a geometrical formalism

Manjeet Mudgil* and Narayanan D. Kurur*

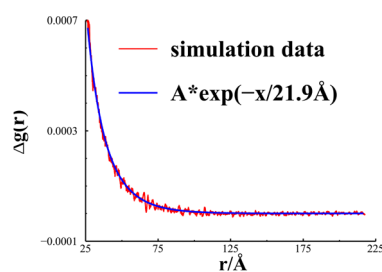


19921

An efficient method to establish electrostatic screening lengths of restricted primitive model electrolytes

Jan Forsman,* David Ribar and Clifford E. Woodward

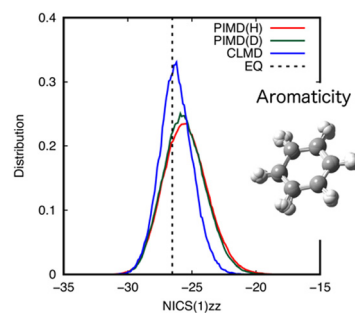
screening length predicted by Widom method: 21.9



19934

Nuclear quantum and H/D isotope effects on aromaticity: path integral molecular dynamics study

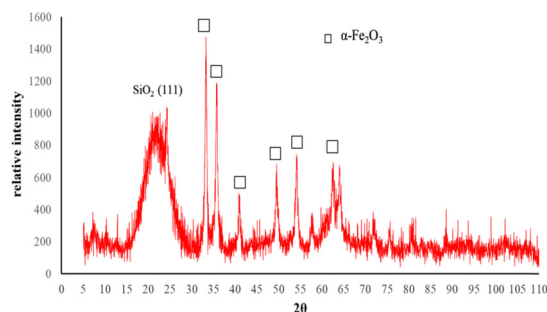
Hikaru Tanaka, Kazuaki Kuwahata, Masanori Tachikawa and Taro Udagawa*



19940

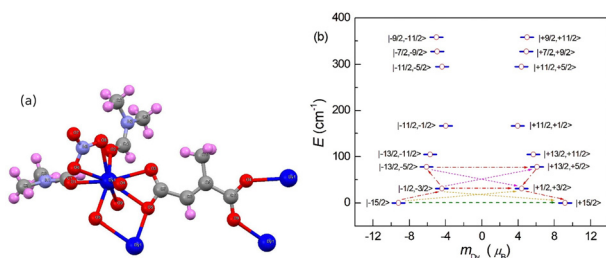
The effect of an external magnetic field on the interaction of carbon monoxide with hematite

P. A. Chernavskii* and G. V. Pankina



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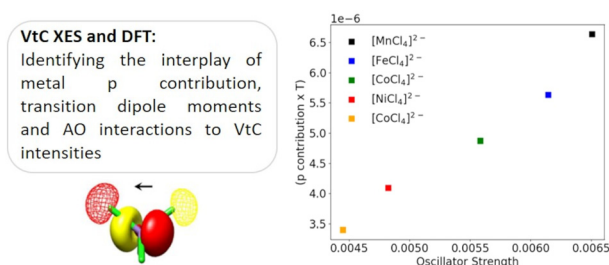
19947



Tailoring single-ion magnet properties of coordination polymer $C_{11}H_{18}DyN_3O_9$ (Dy-CP) using the radial effective charge model (RECM) and superposition model (SPM)

Dinabandhu Halder, Yatramohan Jana,*
Danuta Piwowarska, Paweł Gnutek and
Czesław Rudowicz

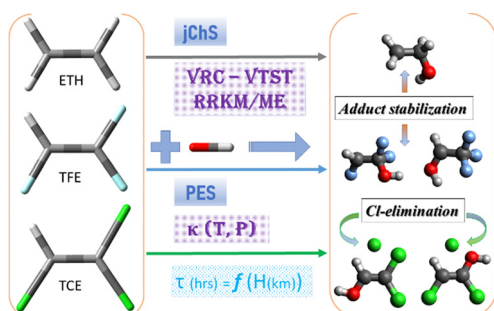
19960



Valence-to-core X-ray emission spectroscopy of transition metal tetrahalides: mechanisms governing intensities

Christina Roemelt, Sergey Peredkov, Frank Neese,
Michael Roemelt* and Serena DeBeer*

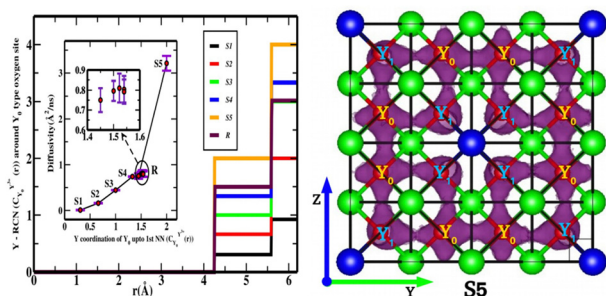
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Theoretical investigation of the OH-initiated atmospheric degradation mechanism of $CX_2=CHX$ ($X = H, F, Cl$) by advanced quantum chemical and transition state theory methods

Nadjib Rais, Zoi Salta* and Nicola Tasinato

19992



Understanding oxide ion transport in cation-ordered yttria-stabilized zirconia

Sudeshna Madhual* and P. Padma Kumar*

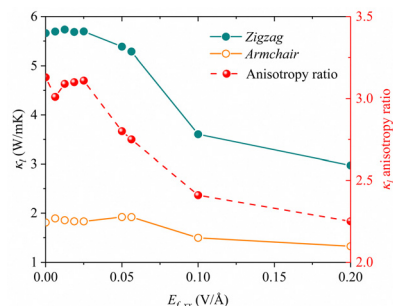


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20000

Giant manipulation of thermal conductivity anisotropy in black phosphorene under external electric fields

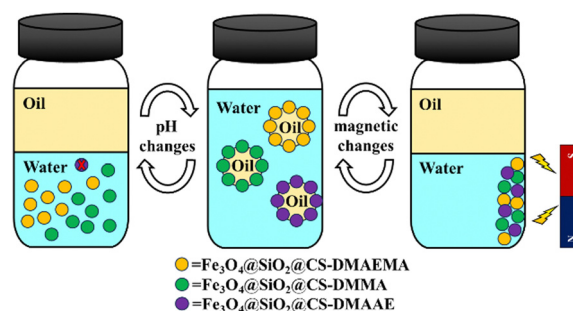
Zhonghua Yang,* Mengyuan Zhang, Wen Gu, Xinyi Xu, Chan Liu and Xinying Lan



20009

Multi-responsive Pickering emulsifiers: a comprehensive study on the emulsification–demulsification behavior of modified chitosan-coated Fe₃O₄ nanocomposites

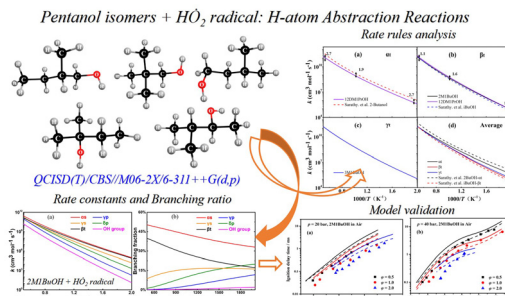
Jianwen Hu, Mingshuo Chi, Runna He, Junjie Fan, Haotian Gao, Wenqing Xie, Kunxiu Dai, Shuangqing Sun* and Songqing Hu*



20022

Theoretical study on the H-atom abstraction reactions of pentanol + HO₂, part I: five branched pentanol isomers

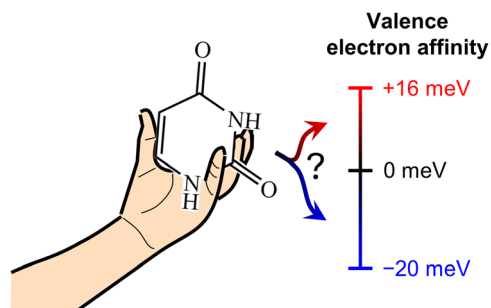
Jin-Tao Chen, Yueying Liang, Haoyuan Lang, Xingcai Lu, Lijun Yang and Chong-Wen Zhou*



20037

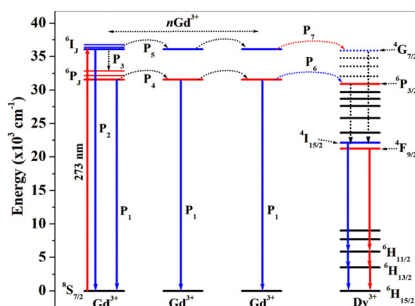
The valence electron affinity of uracil determined by anion cluster photoelectron spectroscopy

Connor J. Clarke, E. Michi Burrow and Jan R. R. Verlet*



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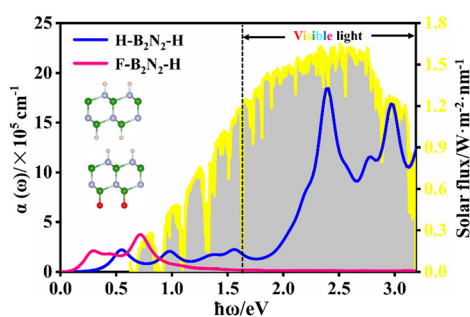
20046



NaGdF₄:Dy³⁺ nanocrystals: new insights into optical properties and energy transfer processes

Vu Xuan Quang, Nguyen Thi Hien, Nguyen Thi Luyen, Nguyen Trung Kien, Nguyen Thi Khanh Van, Nguyen Thi Minh Thuy, Phan Van Do and Nguyen Xuan Ca*

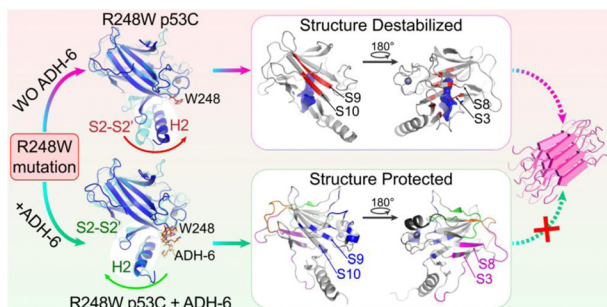
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Functionalized hexagonal boron nitride bilayers: desirable electro-optical properties for optoelectronic applications

Huabing Shu

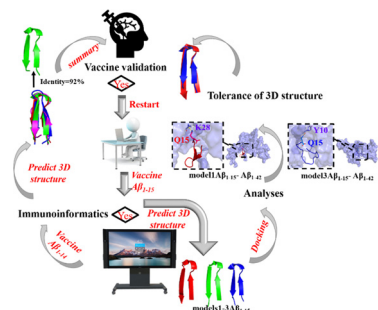
20068



Oncogenic R248W mutation induced conformational perturbation of the p53 core domain and the structural protection by proteomimetic amyloid inhibitor ADH-6

Qian Liu, Yawei Yu and Guanghong Wei*

20087



Prediction of the 3D conformation of a small peptide vaccine targeting Aβ₄₂ oligomers

Yvning Guan, Jinfei Mei, Xvzhi Gao, Chuanbo Wang, Mengke Jia, Sajjad Ahmad, Fahad Nouman Muhammad and Hongqi Ai*

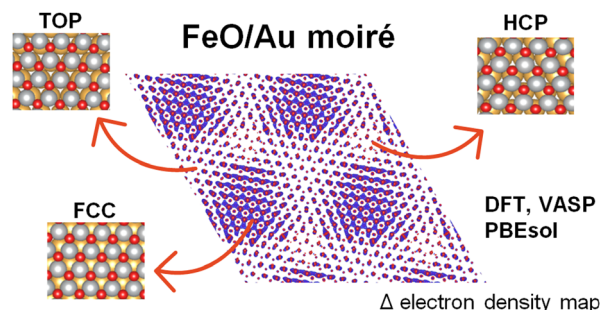


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DFT study of the moiré pattern of FeO monolayer on Au(111)

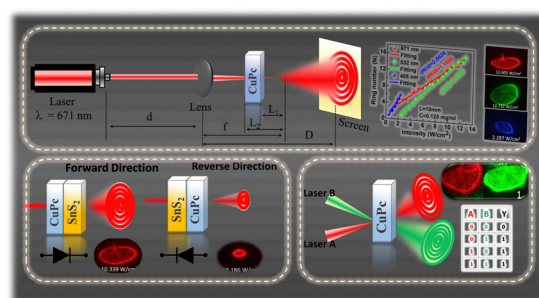
Eleonora Ascrizzi, Jacek Goniakowski, Jijin Yang, Stefano Agnoli and Anna Maria Ferrari*



20112

Strong light–matter interaction and non-linear effects in organic semiconducting CuPc nanotubes: realization of all-optical diode and switching applications

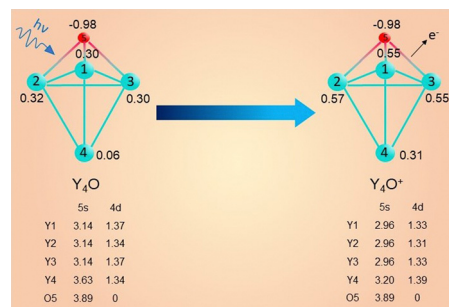
Piyali Dey, Nabamita Chakraborty, Madhupriya Samanta, Biswajit Das and Kalyan Kumar Chattopadhyay*



20123

Structure of small yttrium monoxide clusters, chemical bonding, and photoionization: threshold photoionization and density functional theory investigations

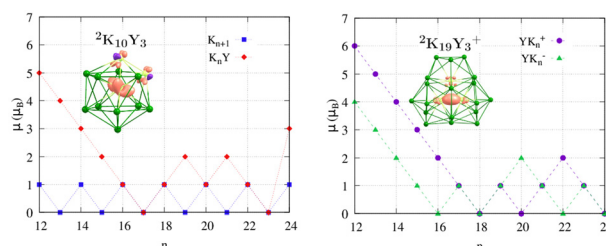
Varun Vinayak Deshpande, Vaibhav Chauhan, Debashis Bandyopadhyay, Anakuthil Anoop and Soumen Bhattacharyya*



20134

On the energetic and magnetic stability of potassium atomic clusters doped by yttrium

Henry Nicole González-Ramírez* and Zeferino Gómez-Sandoval



CORRECTION

20147

Correction: A detailed study of the electronic and optical properties of germanium nanotubes

Hsin-Yi Liu, Yu-Huang Chiu and Jhao-Ying Wu*

