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See David A. Dixon *et al.*, pp. 8355–8368. Image reproduced by permission of David A. Dixon from *Phys. Chem. Chem. Phys.*, 2023, **25**, 8355.

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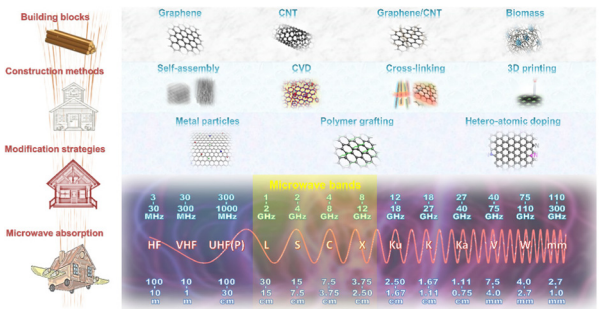
Construction and application of carbon aerogels in microwave absorption

Yifan Guo, Junhua Su, Tongxin Bian, Jing Yan, Longkun Que, Hunan Jiang, Jinlong Xie, Ying Li, Yong Wang and Zuowan Zhou*



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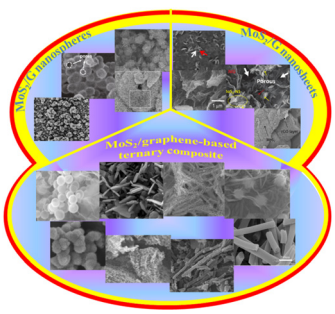
Recent advances in hierarchical MoS_2/graphene-based materials for supercapacitor applications

Ying Ma, Jinchuan Liu, Yinhe Lin* and Yulong Jia*



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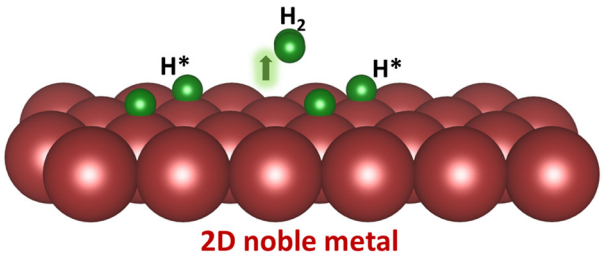
2D noble metals: growth peculiarities and prospects for hydrogen evolution reaction catalysis

Ivan Shtepliuk



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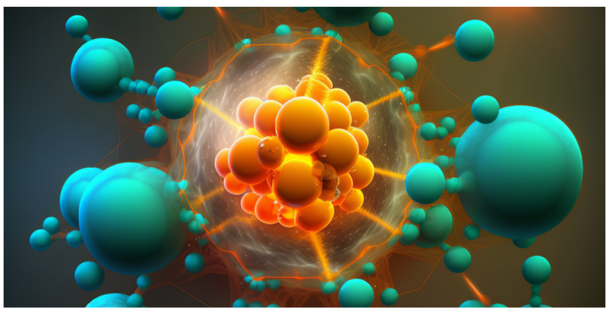
Surface hopping modeling of charge and energy transfer in active environments

Josene M. Toldo,* Mariana T. do Casal, Elizete Ventura, Silmar A. do Monte* and Mario Barbatti*



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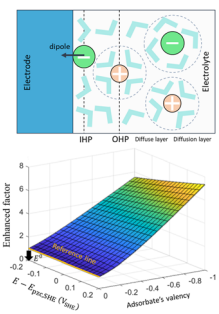
The electrostatic effect and its role in promoting electrocatalytic reactions by specifically adsorbed anions

Wei Chen, Lu-Lu Zhang, Zhen Wei, Meng-Ke Zhang, Jun Cai* and Yan-Xia Chen*



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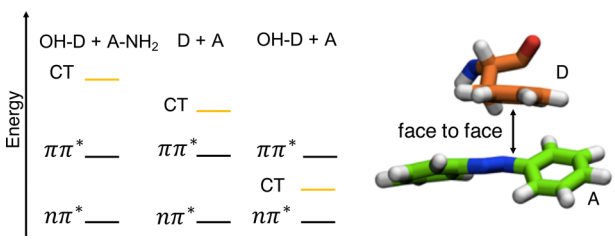
Effect of stacking interactions on charge transfer states in photoswitches interacting with ion channels

Vito F. Palmisano, Shirin Faraji* and Juan J. Nogueira*



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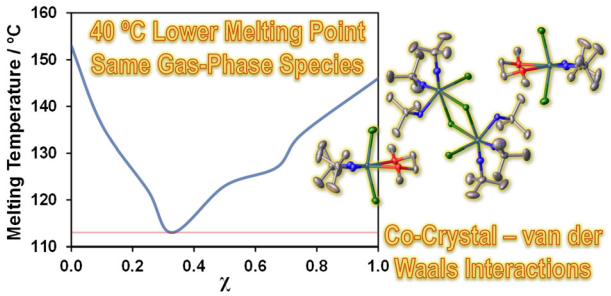

Disturbance of intermolecular forces: eutectics as a new tool for the preparation of vapor-phase deposition precursors

Michael A. Land,* Katherine N. Robertson, Jason A. C. Clyburne and Seán T. Barry

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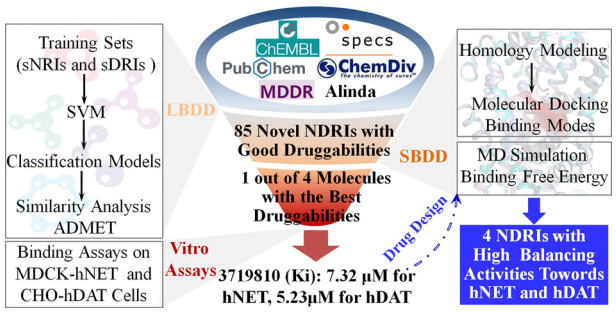

A multiple-step screening protocol to identify norepinephrine and dopamine reuptake inhibitors for depression

Panpan Wang,* Fengmei Yan, Jianghong Dong, Shengqiang Wang, Yu Shi, Mengdan Zhu, Yuting Zuo, Hui Ma, Ruirui Xue, Dingjie Zhai and Xiaoyu Song

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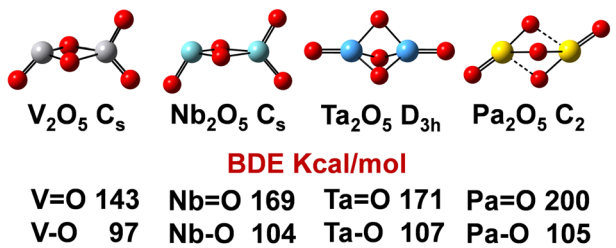

Prediction of the structures and heats of formation of MO_2, MO_3, and M_2O_5 for M = V, Nb, Ta, Pa

Eddy Lontchi, Marcos M. Mason, Monica Vasiliu and David A. Dixon*

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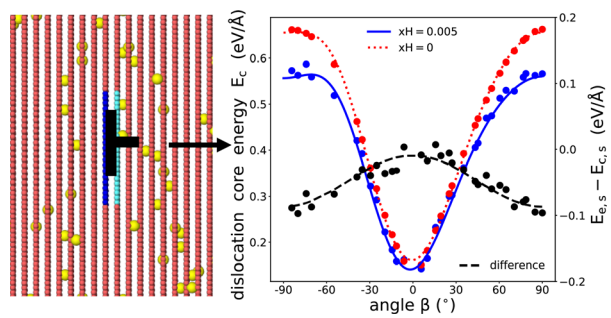

An interplay between a hydrogen atmosphere and dislocation characteristics in BCC Fe from time-averaged molecular dynamics

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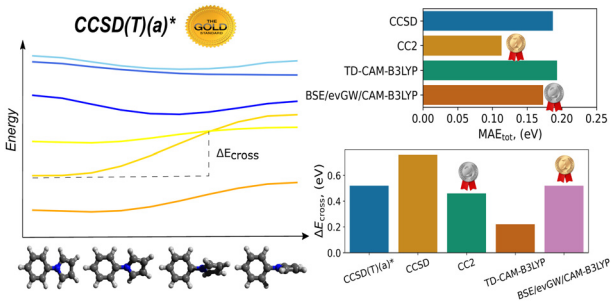
Excited state potential energy surfaces of *N*-phenylpyrrole upon twisting: reference values and comparison between BSE/*GW* and TD-DFT

Iryna Knysh, Kelvine Letellier, Ivan Duchemin, Xavier Blase* and Denis Jacquemin*



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Composition-dependent chemical ordering predicted in Pt–Ag nanoalloys

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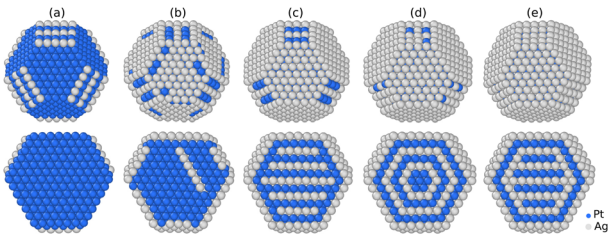

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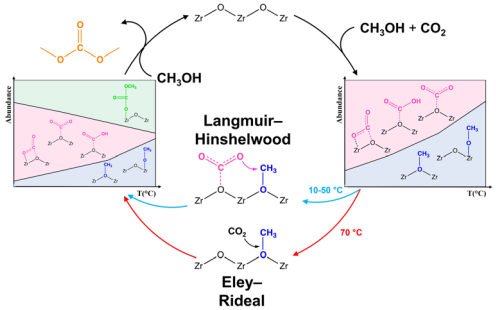
Surface species in direct liquid phase synthesis of dimethyl carbonate from methanol and CO_2: an MCR-ALS augmented ATR-IR study

Matteo Signorile,* Davide Salusso, Valentina Crocellà, Maria Cristina Paganini, Silvia Bordiga, Francesca Bonino and Davide Ferri



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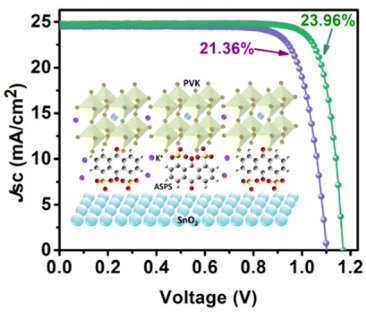
Multifunctional anthraquinone-sulfonic potassium salts passivate the buried interface for efficient and stable planar perovskite solar cells

Yanqiang Hu, Zong Xu, Zhi Wang, Yifan Zhou, Wenwu Song, Yushuang Gao, Guangping Sun, Tongming Sun, Shufang Zhang* and Yanfeng Tang*



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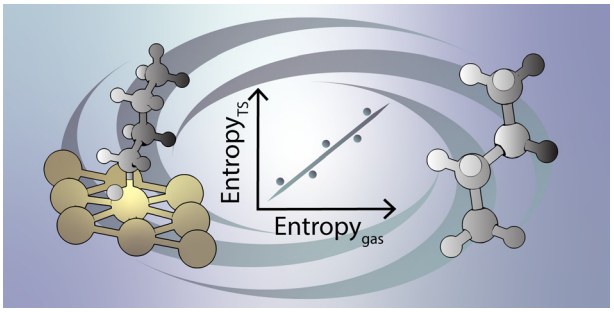

Transition-state correlations for predicting thermochemistry of adsorbates and surface reactions

Sophia J. Kurdziel and Dionisios G. Vlachos*

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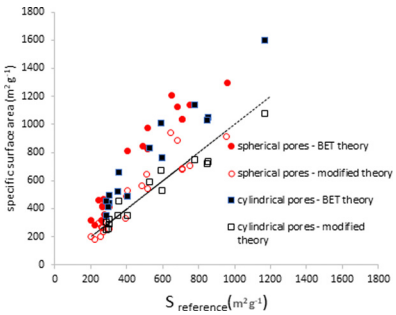

Modified BET theory for actual surfaces: implementation of surface curvature

Behnaz Alinaghipour and Cavus Falamaki*

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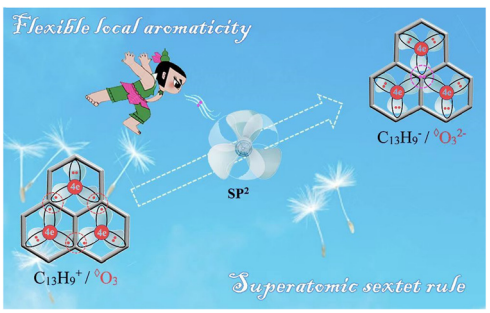

Unraveling the flexible aromaticity of $C_{13}H_9^{+/0/-}$: a 2D superatomic-molecule theory

Dan Li, Chen Yan, Qinqin Yuan,* Lili Shi and Longjiu Cheng*

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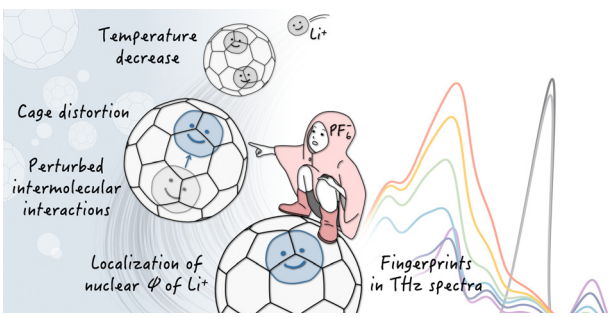

Localization of nuclear wave functions of lithium in $[Li^+@C_{60}]PF_6^-$: molecular insights into two-site disorder–order transition

Hideo Ando* and Yoshihide Nakao

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Structure and formation of copper cluster ions in multiply charged He nanodroplets

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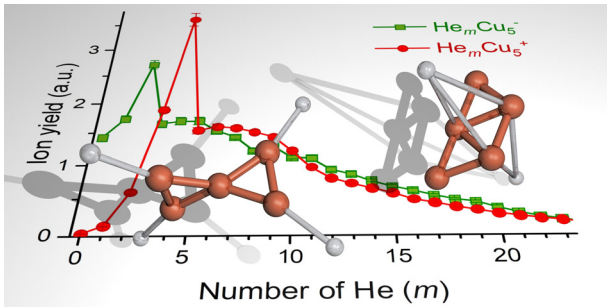

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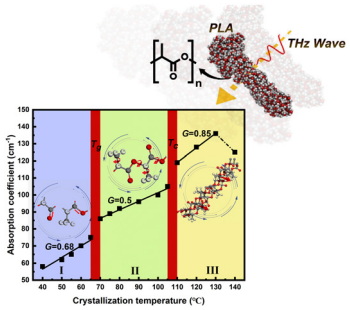
Study on the crystallization behavior and conformation adjustment scale of poly(lactic acid) in the terahertz frequency range

Zhenqi Zhu, Yujing Bian, Xun Zhang, Ruonan Zeng and Bin Yang*



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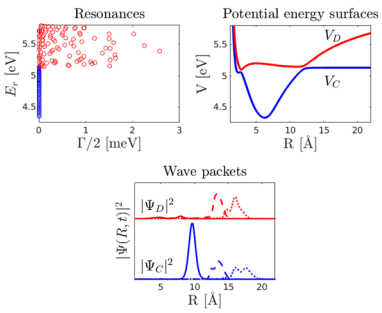
Nonadiabatic wave packet dynamics and predissociation resonances in sodium hydride

Hans O. Karlsson



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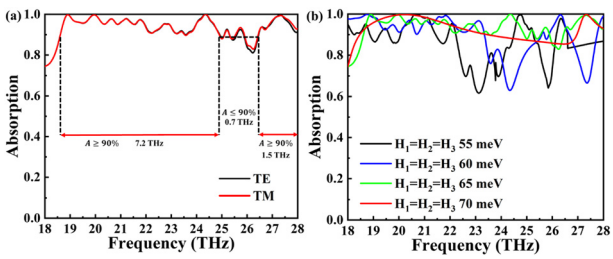
Tunable broadband absorber based on a layered resonant structure with a Dirac semimetal

Wenxin Li, Jing Ma, Huafeng Zhang, Shubo Cheng,* Wenxing Yang,* Zao Yi,* Hua Yang, Jianguo Zhang, Xianwen Wu and Pinghui Wu



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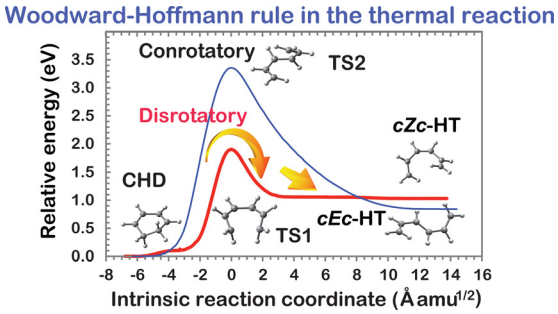

Real-time observation of the Woodward–Hoffmann rule for 1,3-cyclohexadiene by femtosecond soft X-ray transient absorption

Taro Sekikawa,* Nariyuki Saito, Yutaro Kurimoto, Nobuhisa Ishii, Tomoya Mizuno, Teruto Kanai, Jiro Itatani, Kenichiro Saita and Tetsuya Taketsugu

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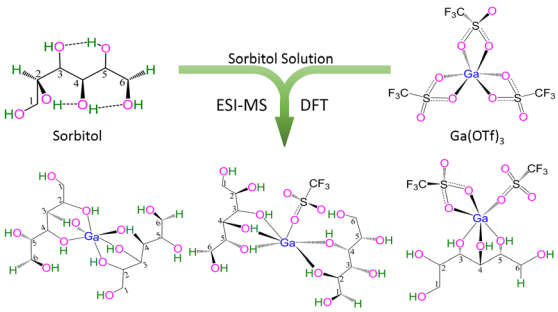
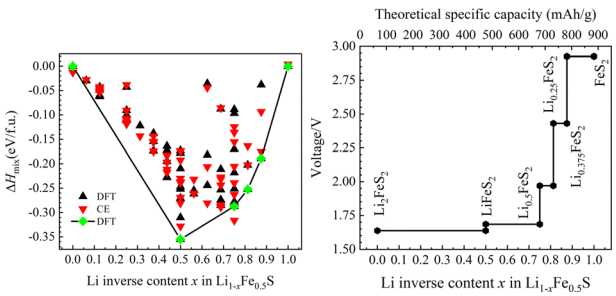


Coordination of sorbitol to $Ga(OTf)_3$ in the liquid phase: an experimental and theoretical study

Mei Li, Jin-Shan Xiong, Han-Yun Min, Ye-Xin Hu, Liang-Fang Zhu, Chang-Wei Hu and Hua-Qing Yang*

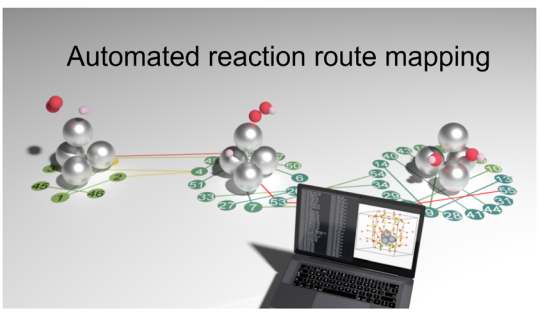
8515



Insights into the electrochemical properties of Li_2FeS_2 after FeS_2 discharging

Cheng-dong Wei, Hong-tao Xue, Xu-dong Zhao and Fu-ling Tang*

8524



An automated reaction route mapping for the reaction of NO and active species on Ag_4 clusters in zeolites

Shunsaku Yasumura, Taisetsu Kato, Takashi Toyao, Zen Maeno and Ken-ichi Shimizu*

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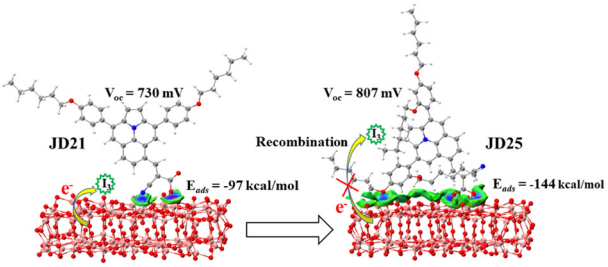
8532

New insights into the alkoxy effects on auxiliary adsorption and inhibiting charge recombination in dye-sensitized solar cells with high open circuit voltage: a theoretical investigation

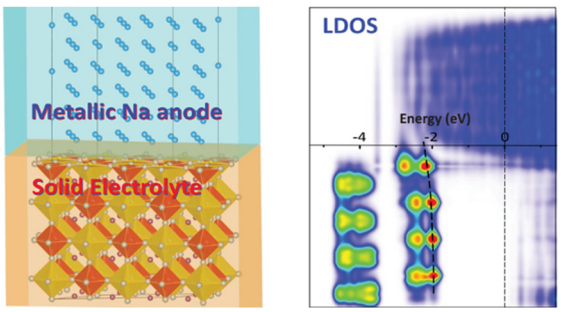
Zi-Han Xu, Chang-Yan Zhu, Xiao-Fei Zhu, Yu-Juan Zhai, Ji Zhang* and Han-Cheng Zhu*



8544

Insight into the structural and electrochemical properties of the interface between a Na_6SOI_2 solid electrolyte and a metallic Na anode

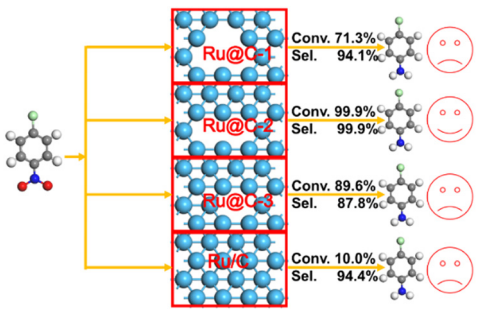
Song-Hyok Choe,* Won-Hyok Hong, Kum-Chol Kim and Chol-Jun Yu*



8556

A well-fabricated Ru@C material derived from Ru/Zn-MOF with high activity and stability in the hydrogenation of 4-chloronitrobenzene

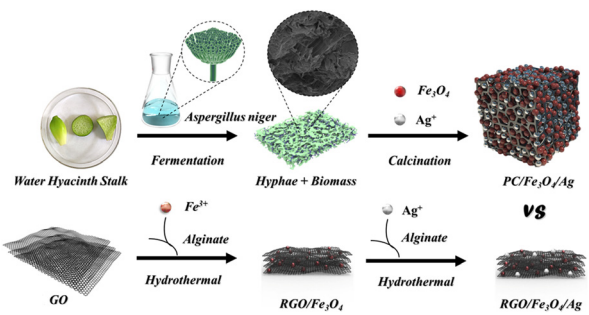
Zijian Wang, Jiaxin Zhang, Lele Yan, Bo Zhao, Lin Zheng, Haoran Guo, Yuxue Yue, Deman Han, Xianlang Chen* and Rongrong Li*



8564

Fungi-enabled pore channel regulation and defect engineering of a novel micro-reactor for treating complex effluents

Xiaoying Jiang, Yan Zhang, Feiyang Zhang, Jiashuo Tian, Liuping Zhang, Xinrui Zhao and Fengling Cui*



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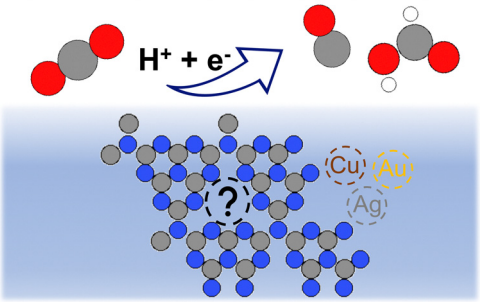
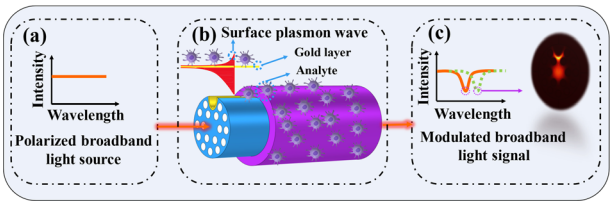
8574



2D carbon nitride as a support with single Cu, Ag, and Au atoms for carbon dioxide reduction reaction

Sergio Posada-Pérez,* Anna Vidal-López, Miquel Solà and Albert Poater*

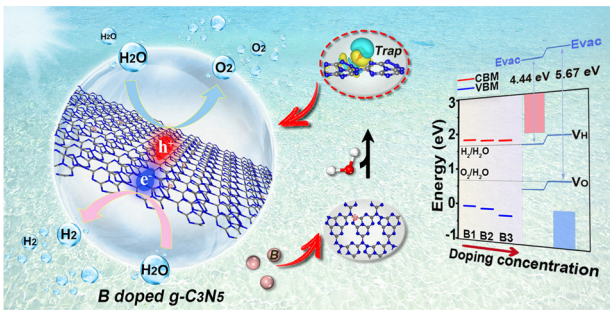
8583



High confidence plasmonic sensor based on photonic crystal fibers with a U-shaped detection channel

Wanlai Zhu, Yingting Yi, Zao Yi,* Liang Bian, Hua Yang, Jianguo Zhang, Yang Yu, Chao Liu, Gongfa Li and Xianwen Wu

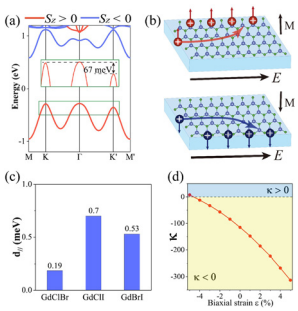
8592



The regulating effect of boron doping and its concentration on the photocatalytic overall water splitting of a polarized g-C_3N_5 material

Xianghong Niu,* Xuemei Zhang, Anqi Shi, Dazhong Sun, Dingbang Chen, Lu Zhang, Jialin Huang, Liqing Liu, Bing Wang* and Xiuyun Zhang*

8600



Combined piezoelectricity, valley splitting and Dzyaloshinskii–Moriya interaction in Janus GdXY (X, Y = Cl, Br, I) magnetic semiconductors

Dehe Zhang, Aolin Li, Bei Zhang, Wenzhe Zhou,* Haiming Duan* and Fangping Ouyang*

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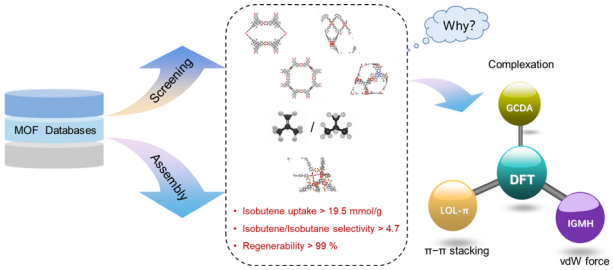
8608

Accelerated screening and assembly of promising MOFs with open Cu sites for isobutene/isobutane separation using a data-driven approach

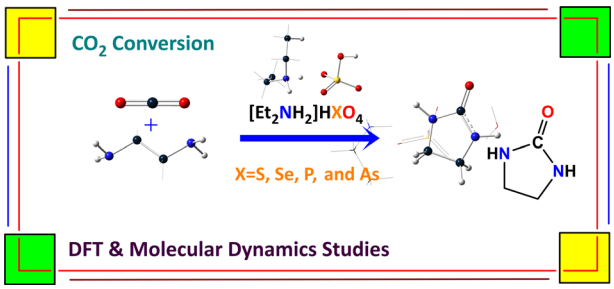
Xi Sun, Wangqiang Lin, Kun Jiang, Heng Liang and Guanghui Chen*



8624

Computational predictions on Brønsted acidic ionic liquid-catalyzed carbon dioxide conversion to five-membered heterocyclic carbonyl derivatives

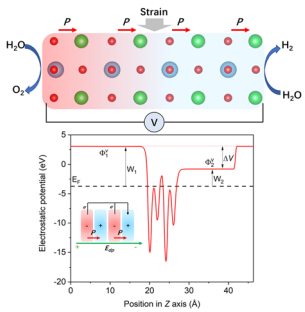
Yusif Abdullayev,* Nazani Karimova, Leonardo A. Schenberg, Lucas C. Ducati and Jochen Autschbach



8631

Understanding the piezocatalytic properties of the $BaTiO_3$(001) surface *via* density functional theory

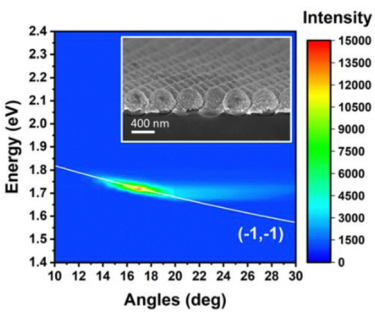
Zeying Zhou, Cheng Zhan* and Erjun Kan



8641

Polarized coherent emission outside high-symmetry points of dye-coupled plasmonic lattices

Diego Piccotti, Mirko Trevisani, Giuseppe Pirruccio, Boris Kalinic, Tiziana Cesca* and Giovanni Mattei



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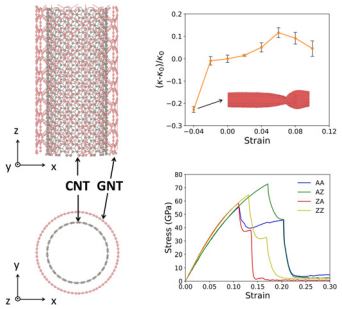
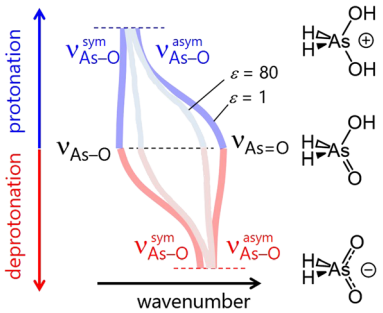


Mechanical and thermal properties of graphyne-coated carbon nanotubes: a molecular dynamics simulation on one-dimensional all-carbon van der Waals heterostructures

Jian Li, Penghua Ying, Ting Liang, Yao Du, Jianli Zhou and Jin Zhang*

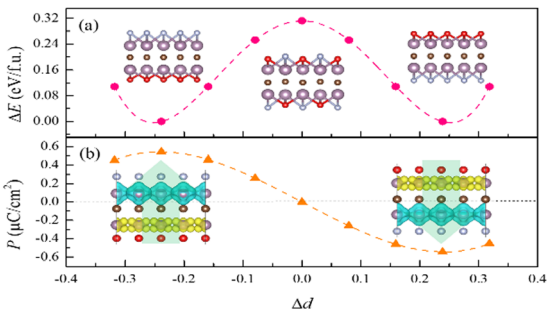
8664



Evolution of vibrational bands upon gradual protonation/deprotonation of arsinic acid $H_2As(O)OH$ in media of different polarity

Elena Yu. Tupikina,* Vladislav O. Korostelev, Danil V. Krutin and Peter M. Tolstoy*

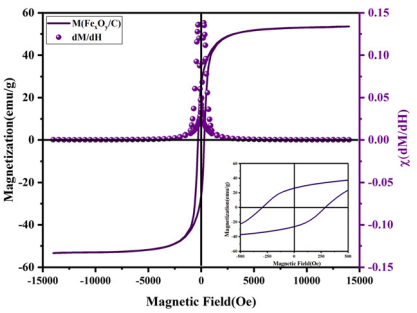
8676



Asymmetric Janus functionalization induced magnetization and switchable out-of-plane polarization in 2D MXene Mo_2CXX'

Chao Xin,* Zhen Fan, Zhixin Sun, Hui Li, Guangyong Jin, Feng Pan* and Yu Sui*

8684



Preparation and characterization study of γ-Fe_2O_3/carbon composite nanofibers: electrospinning of composite fibers using PVP and iron nitrate as precursors

Roya Shokrani Havigh and Hossein Mahmoudi Chenari*

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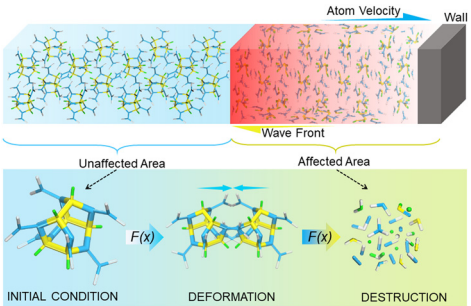
8692

Machine learning quantitatively characterizes the deformation and destruction of explosive molecules

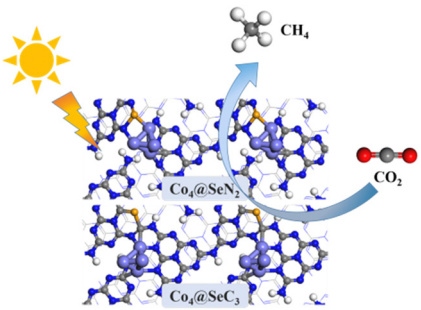
Kaining Zhang, Lang Chen,* Teng Zhang, Jianying Lu, Danyang Liu and Junying Wu



8705

Mechanism of CO_2 photoreduction by selenium-doped carbon nitride with cobalt clusters as cocatalysts

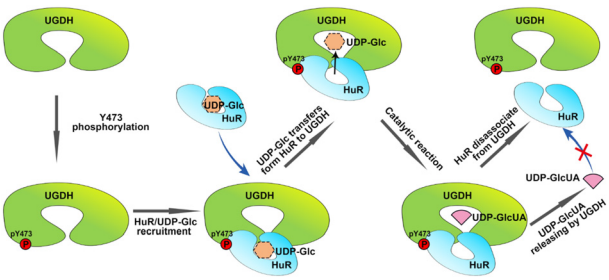
Yuanyuan Hu, Ting Wu, Yi Li, Yongfan Zhang* and Wei Lin*



8714

The molecular mechanism of Y473 phosphorylation of UGDH relieves the inhibition effect of UDP-glucose on HuR

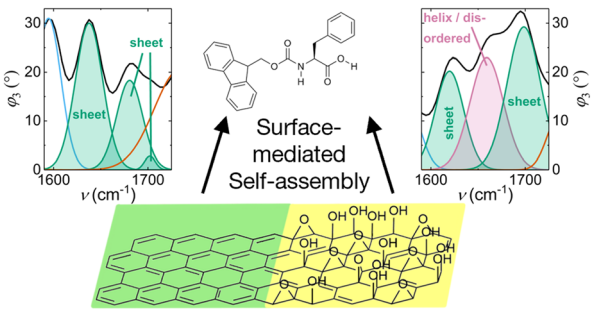
Ye Liu, Yan Li, Guohui Li* and Huiying Chu*



8725

Diversity at the nanoscale: laser-oxidation of single-layer graphene affects Fmoc-phenylalanine surface-mediated self-assembly

Johanna Schirmer, Romain Chevigny, Aleksei Emelianov, Eero Hulkko, Andreas Johansson, Pasi Myllyperkiö, Efstratios D. Sitsanidis,* Maija Nissinen* and Mika Pettersson*



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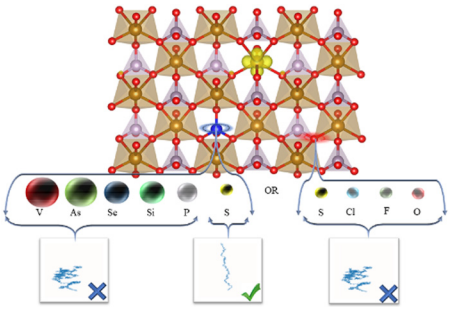
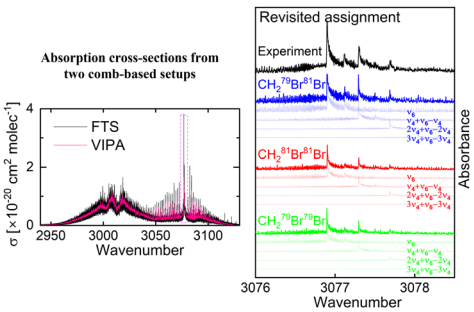


Tuning a small electron polaron in $FePO_4$ by P-site or O-site doping based on DFT+*U* and KMC simulation

Taowen Chen, Yaokun Ye,* Ying Wang, Chi Fang, Weicheng Lin, Yao Jiang, Bo Xu, Chuying Ouyang* and Jiaxin Zheng*

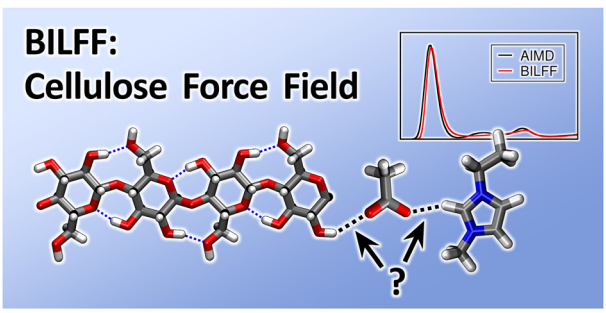
8743



Optical frequency comb-based measurements and the revisited assignment of high-resolution spectra of CH_2Br_2 in the 2960 to 3120 cm^{-1} region

Ibrahim Sadiek,* Adrian Hjältén, Frances C. Roberts, Julia H. Lehman and Aleksandra Foltynowicz

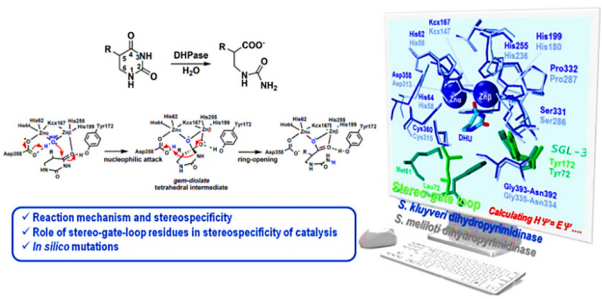
8755



A force field for bio-polymers in ionic liquids (BILFF) – part 2: cellulose in [EMIm][OAc]/water mixtures

Eliane Roos, Daniel Sebastiani and Martin Brehm*

8767



A computational study of the reaction mechanism and stereospecificity of dihydropyrimidinase

Wijitra Meelua, Tanchanok Wanjai, Natechanok Thinkumrob, Julianna Oláh, James R. Ketudat Cairns, Supa Hannongbua, Ulf Ryde and Jitrayut Jitonnom*

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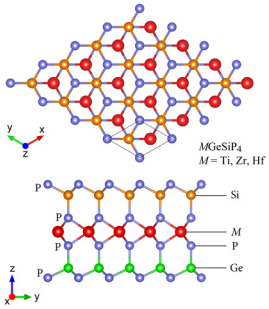
8779

Two-dimensional Janus $MGeSiP_4$ (M = Ti, Zr, and Hf) with an indirect band gap and high carrier mobilities: first-principles calculations

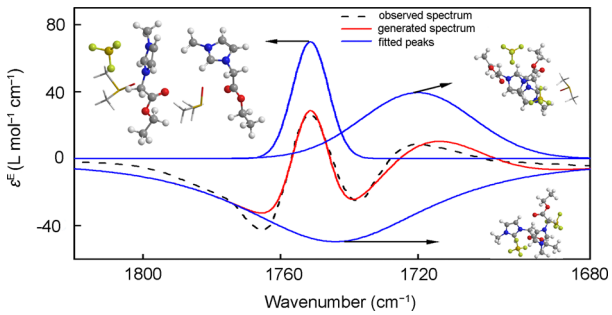
Nguyen T. Hiep, Nguyen P. Q. Anh, Huynh V. Phuc, Cuong Q. Nguyen, Nguyen N. Hieu and Vo T. T. Vi*



8789

Comparative study of the hydrogen bonding interactions between ester-functionalized/non-functionalized imidazolium-based ionic liquids and DMSO

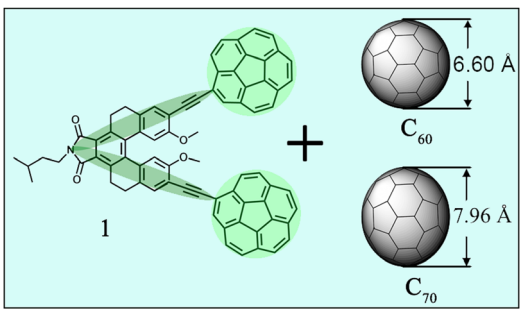
Yuxin Jiang, Xianzhen Xu, Mingzhu Wang, Yu Zhou* and Zonghua Wang*



8799

Effect of intermolecular interaction of the charge-transfer complex between molecular "tweezers" and C_{60}/C_{70} on second-order nonlinear optical properties

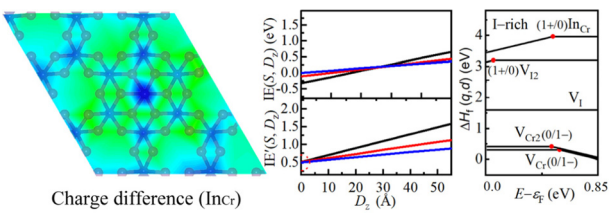
Li Wang,* Yan-Li Liu, Quan-Jiang Li, Di He, Sheng-Hui Chen and Mei-Shan Wang*



8809

Electronic and magnetic properties of charged point defects in monolayer CrI_3

Rongrong Ma, Yun Sun, Mei Ge, Chenrui Ma and Junfeng Zhang*



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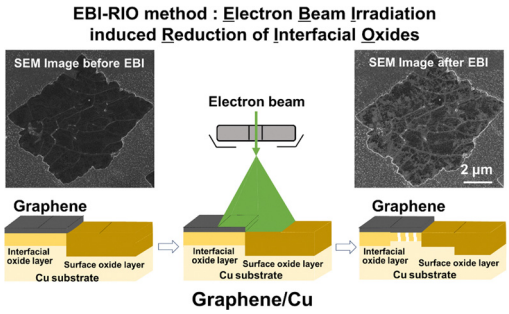
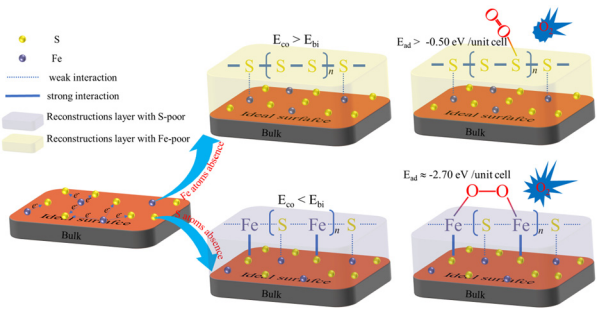


Nanoscale characterization of the heterogeneous interfacial oxidation layer of graphene/Cu based on a SEM electron beam induced reduction effect

Panpan Feng, Dan Zhang,* Peng Zhang, You Wang and Yang Gan*

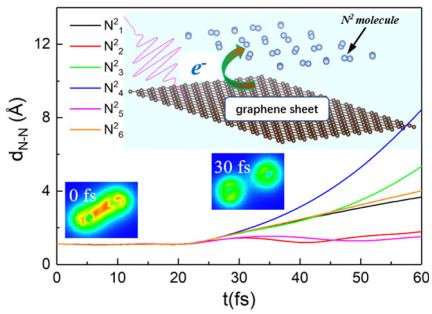
8826



Atomic reconstruction and oxygen adsorption behavior of the pyrite (100) surface: a DFT study

Manjiao Chen, Xinjun Hu, Xinjun Zhou, Xiulan Li and Jianping Tian

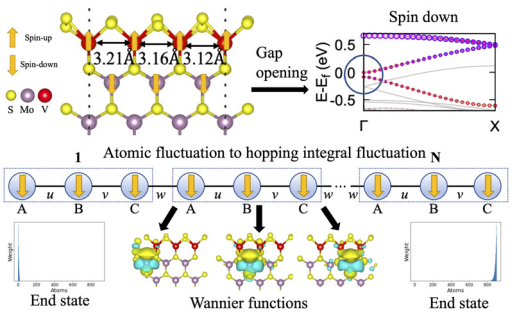
8836



Real-time dynamic simulation of laser-induced N_2 dissociation on two-dimensional graphene sheets

Jiuhuan Chen, Xin-Lu Cheng* and Hong Zhang

8843



Realization of quasi-1D topological magnetism at the V-alloyed MoS_2 zigzag edge

Kejie Bao and Junyi Zhu*

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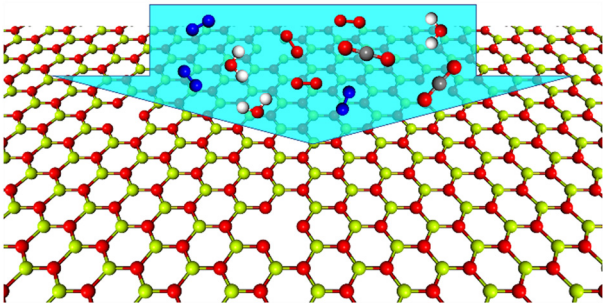
Robust electronic properties of monolayer BeO against molecule adsorption

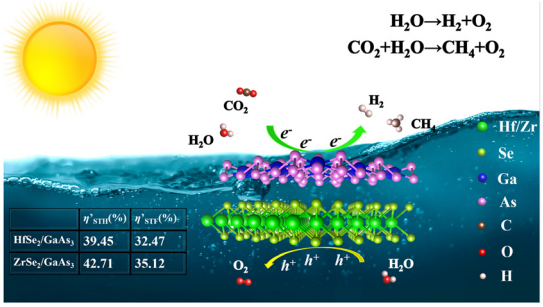
Hongsheng Liu, Vitaly Ksenevich, Jijun Zhao and Junfeng Gao*



8861

Efficient photocatalytic hydrogen evolution and CO_2 reduction by $HfSe_2/GaAs_3$ and $ZrSe_2/GaAs_3$ heterostructures with direct Z-schemes

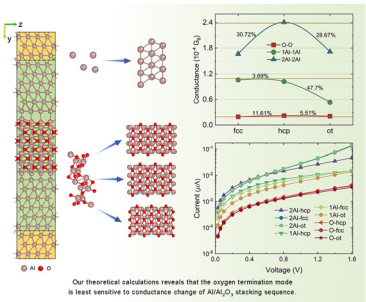
Xue-Qing Wan, Chuan-Lu Yang,* Mei-Shan Wang and Xiao-Guang Ma



8871

Effect of the Al/AlO_x interfacial stacking sequence on the transport properties of alumina tunnel junctions

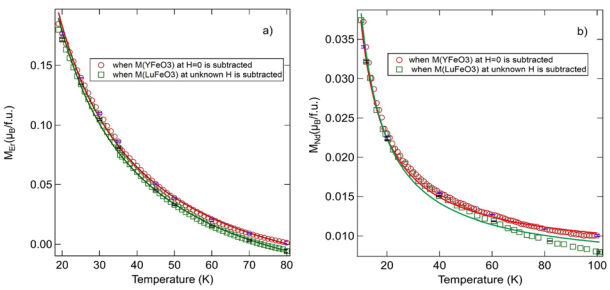
Zheng Shan, Xuelian Gou, Huihui Sun,* Fudong Liu, Lin Han and Jiandong Shang



8882

Temperature dependence of magnetic moment of rare earth ions in $ErFeO_3$ and $NdFeO_3$ single crystals

Mohanad H. Mohammed, Zhenxiang Cheng, Shixun Cao and Joseph Horvat



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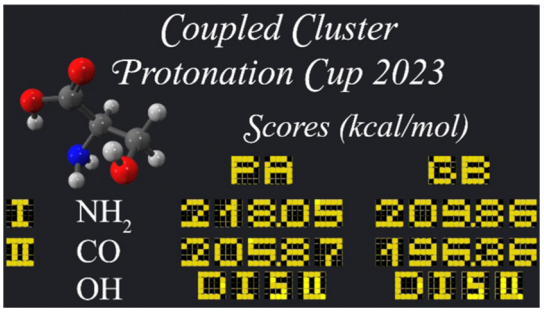
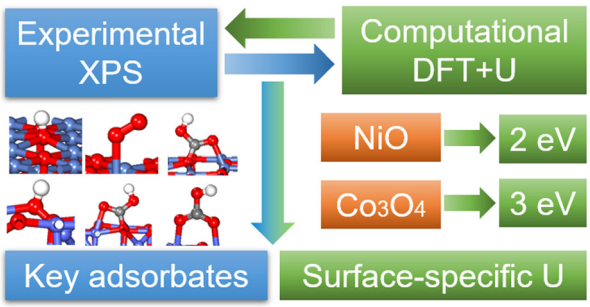


Protonation of serine: conformers, proton affinities and gas-phase basicities at the "gold standard" and beyond

András B. Nacsa,* Máté Kígyósi and Gábor Czakó*

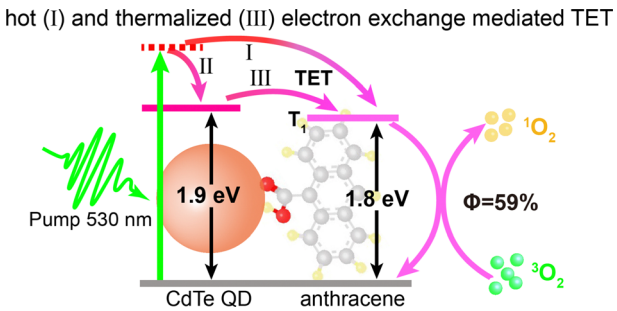
8903



Determining surface-specific Hubbard-*U* corrections and identifying key adsorbates on nickel and cobalt oxide catalyst surfaces

Shang Jiang and Samir H. Mushrif*

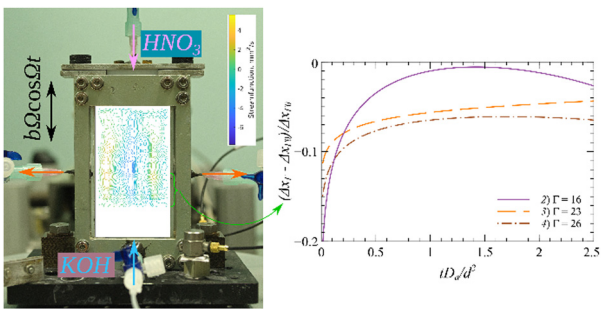
8913



Triplet generation at the CdTe quantum dot/anthracene interface mediated by hot and thermalized electron exchange for enhanced production of singlet oxygen

Zhen Chi, Jia Xu, Shida Luo, Xia Ran, Xiaojuan Wang, Pingan Liu,* Yulu He, Yanmin Kuang and Lijun Guo*

8921



Investigation of chemoconvection in vibration fields

Nikolai Kozlov* and Elena Mosheva

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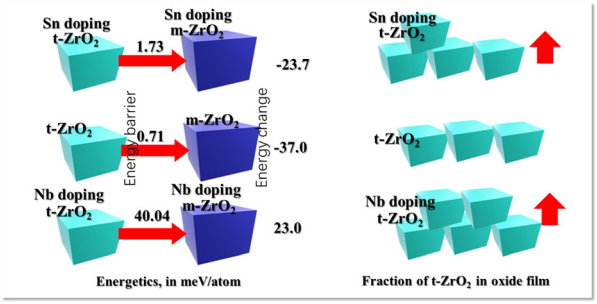
Unraveling different influences of the fraction of the tetragonal phase in oxide films on the corrosion resistance of Zr alloys from the phase transition mechanism

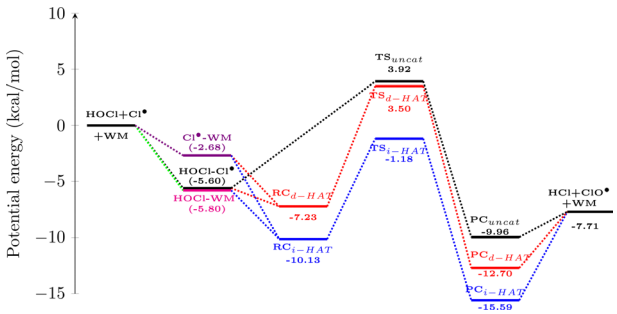
Jiang-Wei Wu, Yao-Ping Xie,* Mei-Yi Yao, Shu-Hui Guan, Yi Zhao, Rong-Jian Pan, Lu Wu and Zhi-Pan Liu



8948

Effect of $(H_2O)_n$ (n = 1 and 2) on HOCl + Cl reaction

Amit Kumar and Pradeep Kumar*

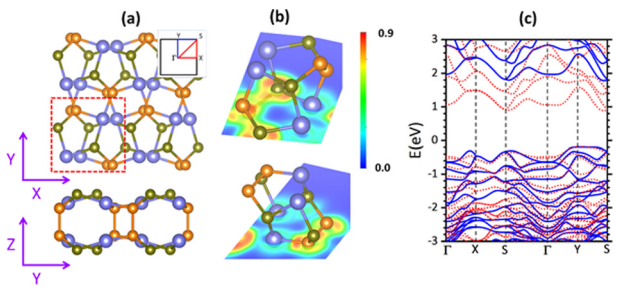


COMMENTS

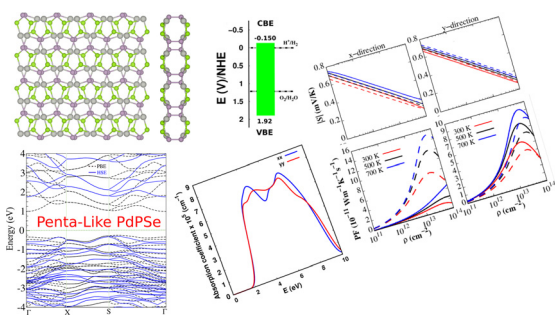
8961

Comment on "Two-dimensional penta-like PdPSe with a puckered pentagonal structure: a first-principles study" by A. Bafekry, M. M. Fadlallah, M. Faraji, A. Shafique, H. R. Jappor, I. Abdolhoseini Sarsari, Y. S. Ang and M. Ghergherehchii, *Phys. Chem. Chem. Phys.*, 2022, 24, 9990

Suman Chowdhury, Fazel Shojaei and Bohayra Mortazavi*



8966

Reply to the 'Comment on "Two-dimensional penta-like PdPSe with a puckered pentagonal structure: a first-principles study"' by S. Chowdhury, F. Shojaei and B. Mortazavi, *Phys. Chem. Chem. Phys.*, 2023, 25, DOI: 10.1039/D2CP01587K

Asadollah Bafekry,* Mohamed M. Fadlallah, Mehrdad Faraji, A. Shafique, Hamad R. Jappor, I. Abdolhoseini Sarsari, Yee Sin Ang and Mitra Ghergherehchi