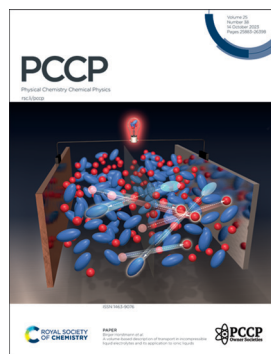


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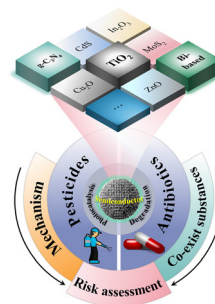
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REVIEW

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Recent advances of semiconductor photocatalysis for water pollutant treatment: mechanisms, materials and applications

Huasheng Wu, Lingxiangyu Li, Sen Wang, Nali Zhu, Zhigang Li, Lixia Zhao* and Yawei Wang

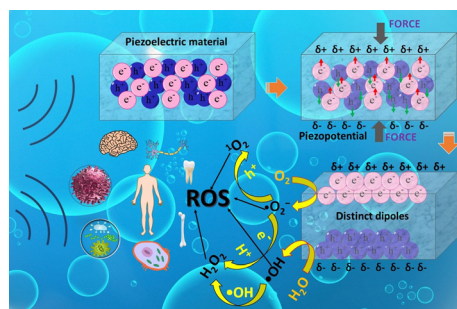


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Reactive oxygen species for therapeutic application: Role of piezoelectric materials

Dipankar Sengupta, Sudip Naskar and Dipankar Mandal*



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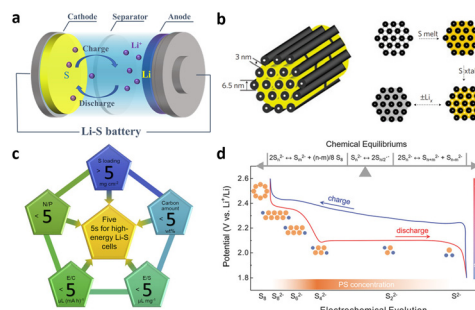


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Single-atom site catalysis in Li–S batteries

Kun Wang, Sheng Liu, Zhenghao Shu, Qingyi Zheng, Mingsen Zheng* and Quanfeng Dong*

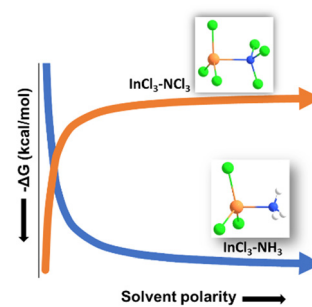


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Trends in the stability of covalent dative bonds with variable solvent polarity depend on the charge transfer in the Lewis electron-pair system

Rabindranath Lo, Debashree Manna, Vijay Madhav Miriyala, Dana Nachtigallová and Pavel Hobza*

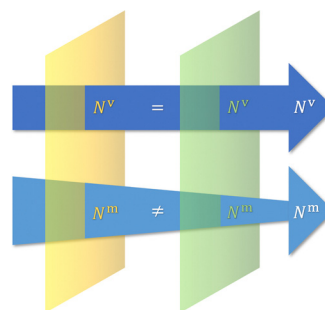


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A volume-based description of transport in incompressible liquid electrolytes and its application to ionic liquids

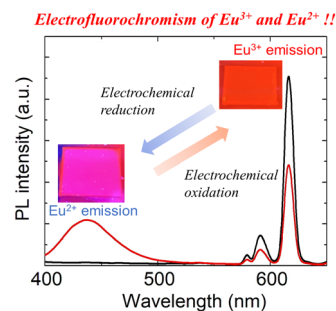
Franziska Kilchert, Martin Lorenz, Max Schammer, Pinchas Nürnberg, Monika Schönhoff, Arnulf Latz and Birger Horstmann*



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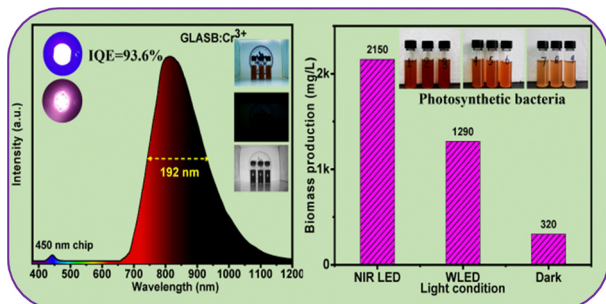
Electrochemically regulated luminescence of europium complexes with β -diketone in polyether matrices

Ryoto Yabuta, Norihisa Kobayashi and Kazuki Nakamura*



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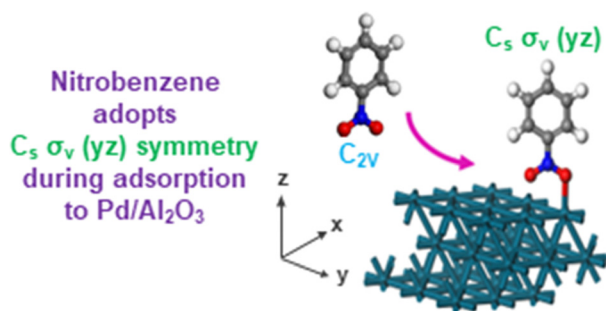
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Highly efficient near-infrared solid solution phosphors with excellent thermal stability and tunable spectra for pc-LED light sources toward NIR spectroscopy applications

Tianchun Lang,* Qunyang Zhao, Xiaolong Jing, Gaoxuanyu Guan, Shuangqiang Fang,* Qinqing Qiang, Lingling Peng, Tao Han, Alexey N. Yakovlev and Bitao Liu*

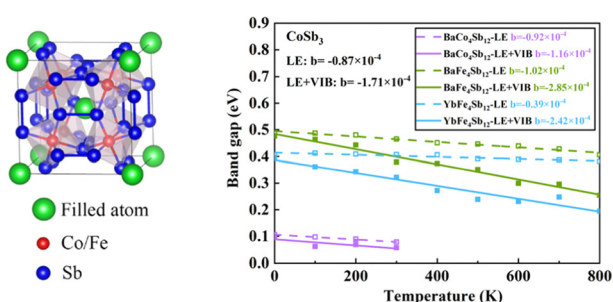
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The adsorption of nitrobenzene over an alumina-supported palladium catalyst: an infrared spectroscopic study

Annelouise M. McCullagh, Emma K. Gibson, Stewart F. Parker, Keith Refson and David Lennon*

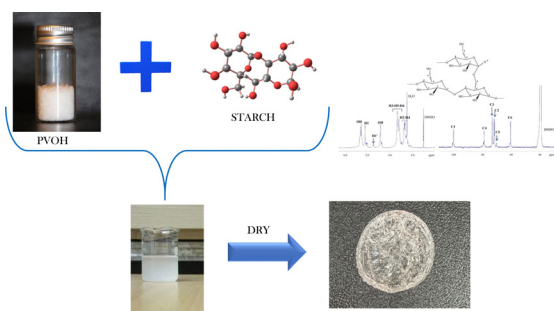
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First-principles study of the temperature-induced band renormalization in thermoelectric filled skutterudites

Jinyan Ning, Wenxin Lei, Jiong Yang* and Jinyang Xi*

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Starch/PVOH aqueous solutions: a chemical–physical characterization

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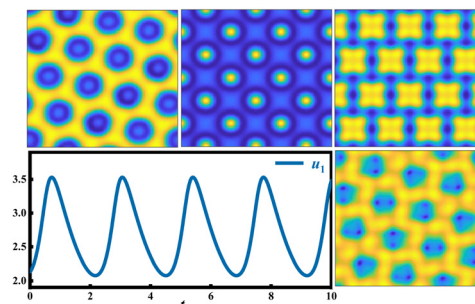


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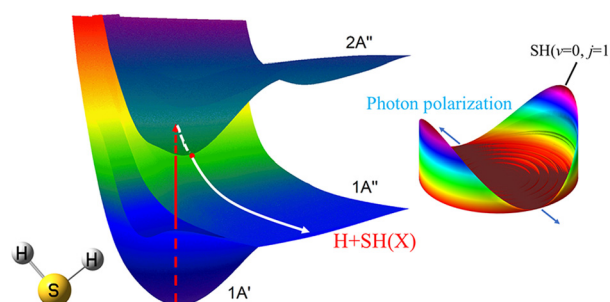
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New accurate diabatic potential energy surfaces for the two lowest $1A''$ states of H_2S and photodissociation dynamics in its first absorption band

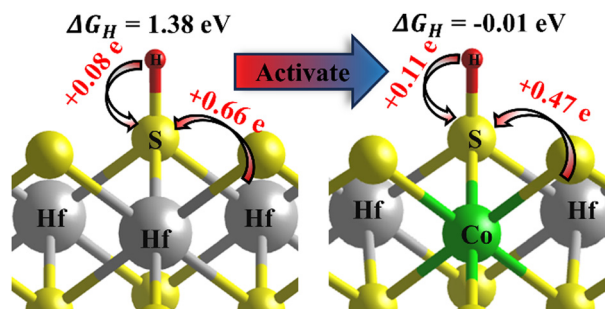
Junjie Chen, Hanzi Zhang, Linsen Zhou,* Xixi Hu* and Daiqian Xie



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Activating HfX_2 ($X = S, Se$ and Te) for the hydrogen evolution reaction by introducing defects: a first-principles study

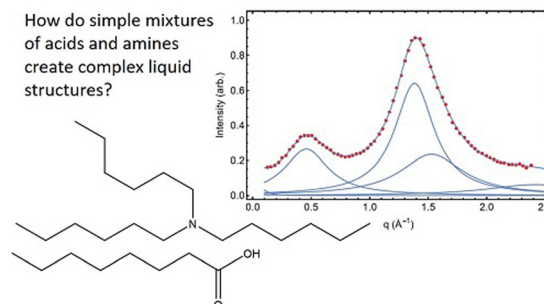
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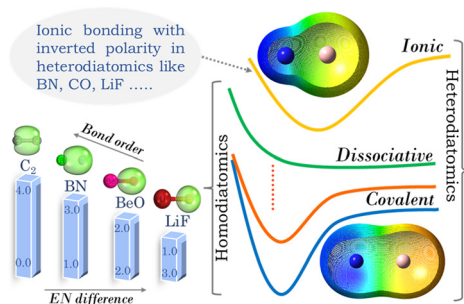
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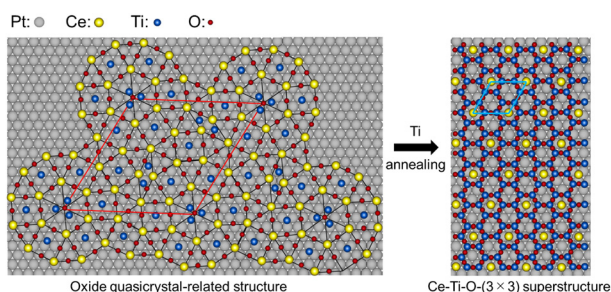
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Eliminating all bonds from the ground state gives rise to ionic bonding in high-spin states of heterodiatomics

Ishita Bhattacharjee, Debashree Ghosh* and Ankan Paul*

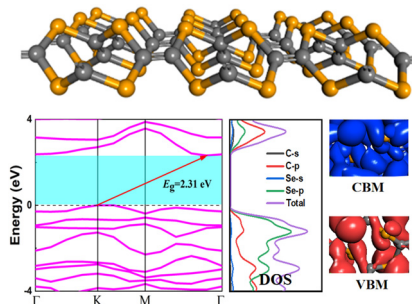
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Growth of a quasicrystal-related structure and superstructure for ultrathin Ce–Ti–O films on Pt(111)

Xu Li,* Lap Hong Chan, Sho-ichi Takakura, Masashi Nakatake, Tsunetomo Yamada, Ryuji Tamura and Junji Yuhara

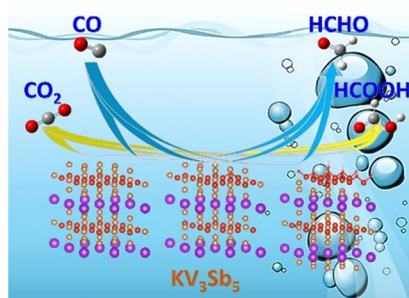
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Designing novel monolayer and multilayer h-CSe crystals with tunable photoelectric properties

Xiumei Dong, Caixia Mao, Libing Qian,* Yonghong Hu,* Li Xue and Haiming Huang*

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Surface-independent CO₂ and CO reduction on two-dimensional kagome metal KV₃Sb₅

Xin-Wei Chen, Zheng-Zhe Lin* and Meng-Rong Li

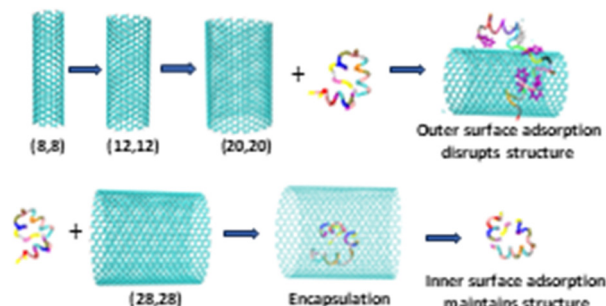


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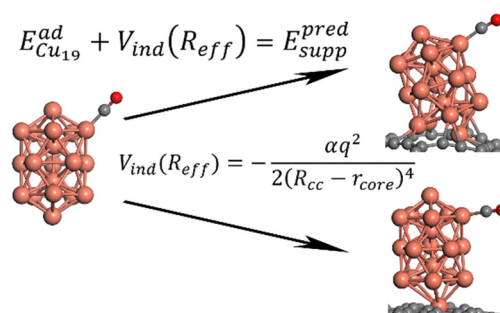
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Enhanced CO adsorption on α -graphyne-supported and defective graphene-supported Cu_{19} clusters and a modified induction energy model

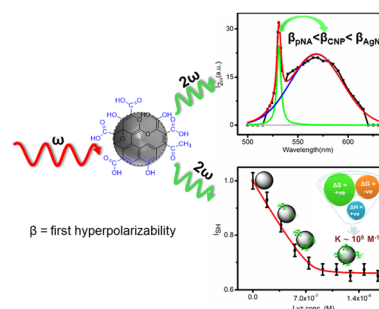
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Lysozyme adsorption on carbonaceous nanoparticles probed by second harmonic light scattering

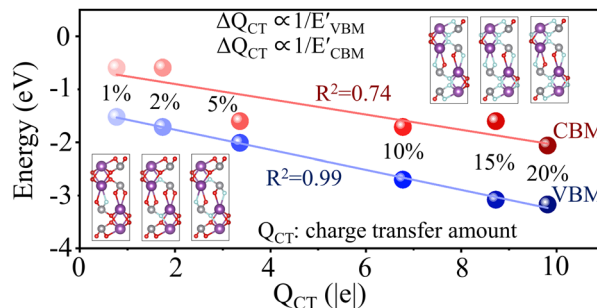
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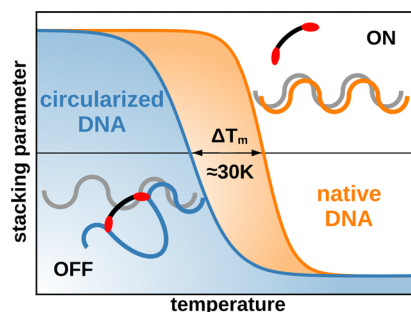
n-Type doping of BiVO_4 with different F-doped concentrations for improving the electronic character of BiVO_4 as a photoanode nanomaterial for solar water splitting: a first-principles study

Yongze Zhao, Xinxia Li, Xinyuan Tang, Xuefeng Liang, Yan He and Hui Fang Li*



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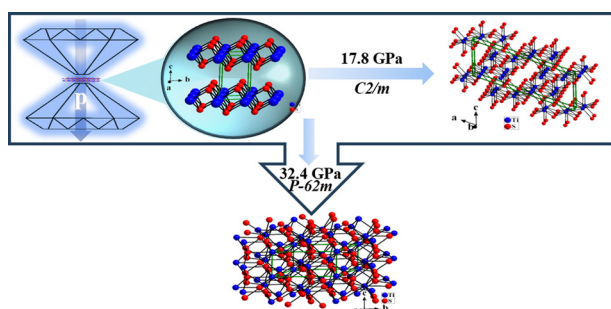
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Controlled destabilization of caged circularized DNA oligonucleotides predicted by replica exchange molecular dynamics simulations

Carsten Hamerla, Padmabati Mondal, Rainer Hegger and Irene Burghardt*

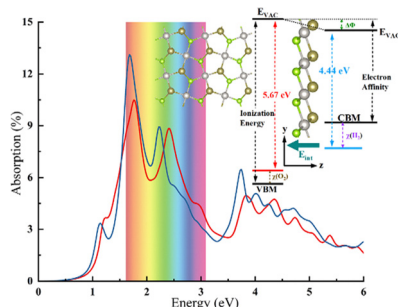
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Pressure-modulated lattice structural evolution in TiS_2

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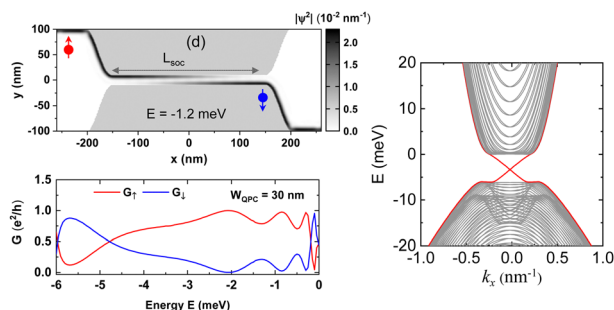
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Two-dimensional Janus pentagonal MSeTe ($\text{M} = \text{Ni}, \text{Pd}, \text{Pt}$): promising water-splitting photocatalysts and optoelectronic materials

Yu-Xun Yuan, Lu Pan, Zhao-Qi Wang,* Zhao-Yi Zeng,
Hua-Yun Geng and Xiang-Rong Chen*

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Spin polarization in quantum point contact based on wurtzite topological quantum well

Xin Xue, Fobao Huang and Gongwei Hu*

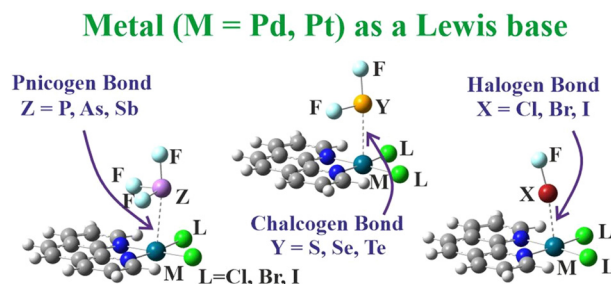


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Pd and Pt metal atoms as electron donors in σ -hole bonded complexes

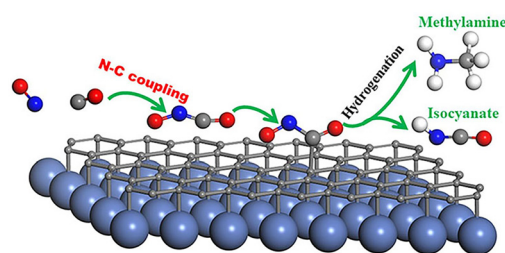
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Insight into the mechanism of direct N–C coupling in selective catalytic reduction of NO by CO over Ni(111)-supported graphene

Tiantian Liu, Juan Wei, Pengfei Liu, Hui Shi,* Qiang Wang* and Yanhui Yang

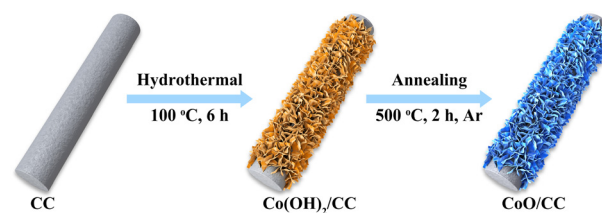


A novel mechanism of direct N-C coupling of NO and CO

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Enhanced hydrogen evolution reaction *via* regulating the adsorbability between 2D CoO nanosheets and CC substrate

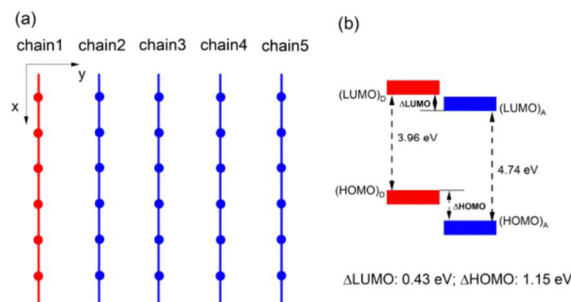
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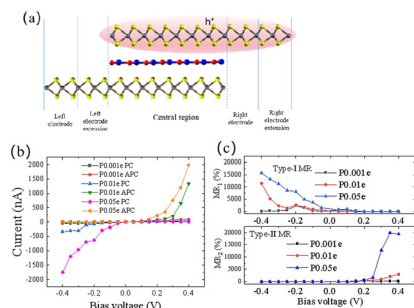
Surface hopping simulations on charge separation in an organic donor–acceptor system

Zhen Sun,* Sheng Li, Shijie Xie, Yan Meng and Zhong An*



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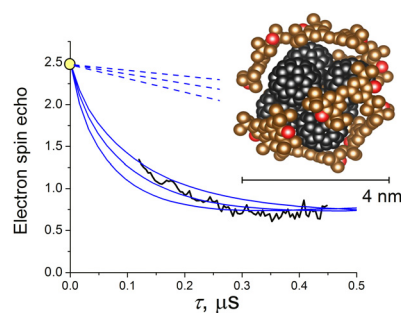
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Reconfigurable spin tunnel diodes by doping engineering VS₂ monolayers

Sheng Yu, Wenwu Shi, Qiliang Li, Feixiang Xu, Li Gu* and Xinzhong Wang*

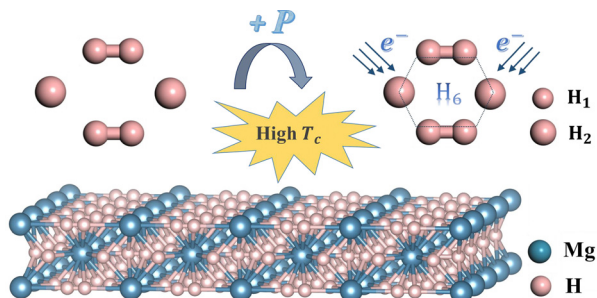
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Assembly of galvinoxyl doped in polymer–fullerene photovoltaic blends

Mikhail N. Uvarov, Leonid V. Kulik and Sergei A. Dzuba*

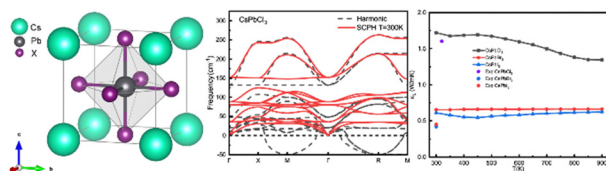
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Composition and structural characteristics of compressed alkaline earth metal hydrides

Ya-Le Tao, Wei Zeng, Juan Gao, Zheng-Tang Liu, Zhen Jiao* and Qi-Jun Liu*

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Anharmonic phonon renormalization and thermoelectric properties of CsPbX₃ (X = Cl, Br, and I): first-principles calculations

Ziang Yao, Wei Cao, Ziyu Wang,* Ling Miao, Jing Shi and Rui Xiong*

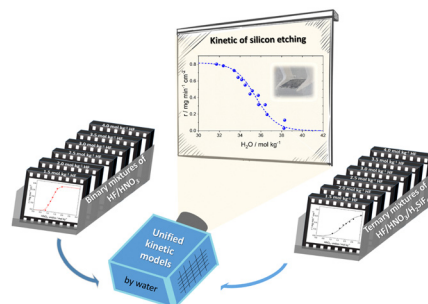


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Kinetic studies on acidic wet chemical etching of silicon in binary and ternary mixtures of HF, HNO₃ and H₂SiF₆

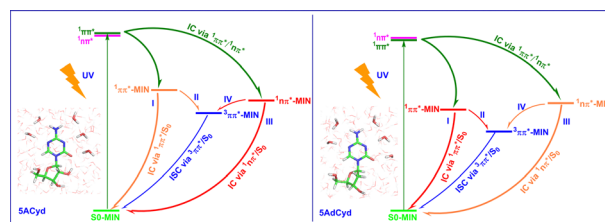
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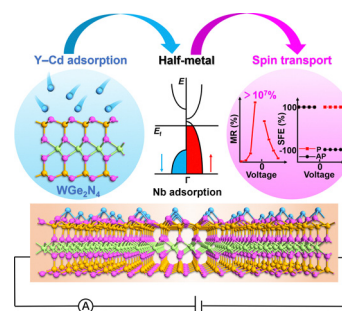
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26270

Regulating the electronic properties of the WGe₂N₄ monolayer by adsorption of 4d transition metal atoms towards spintronic devices

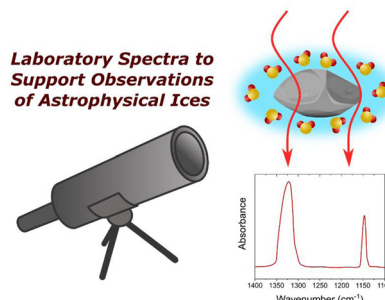
Jin-Lan Sun, Mi-Mi Dong, Yue Niu, Zong-Liang Li, Guang-Ping Zhang, Chuan-Kui Wang* and Xiao-Xiao Fu*



26278

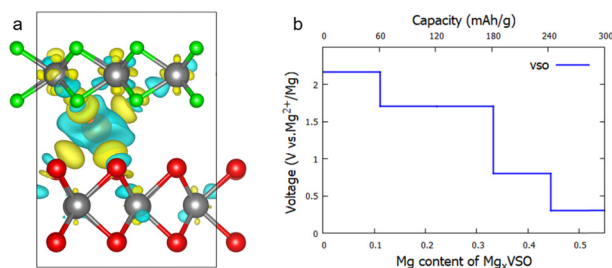
A systematic mid-infrared spectroscopic study of thermally processed SO₂ ices

Duncan V. Mifsud,* Péter Herczku, K. K. Rahul, Ragav Ramachandran, Pavithraa Sundararajan, Sándor T. S. Kovács, Béla Sulik, Zoltán Juhász, Richárd Rácz, Sándor Biri, Zuzana Kaňuchová, Robert W. McCullough, Bhalamurugan Sivaraman, Sergio Ioppolo and Nigel J. Mason*



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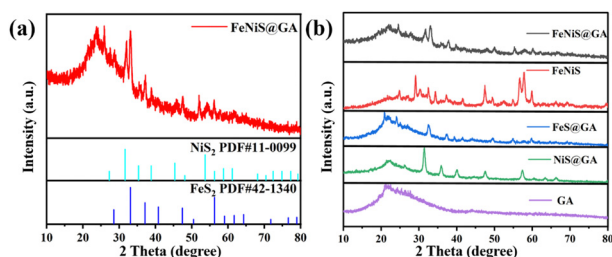
26289



A two-dimensional VO₂/VS₂ heterostructure as a promising cathode material for rechargeable Mg batteries: a first principles study

Lingxiao Luo, Shuangshuang Tan,* Zhipeng Gao, Xiaofang Yang,* Junyao Xu, Guangsheng Huang, Jingfeng Wang and Fusheng Pan

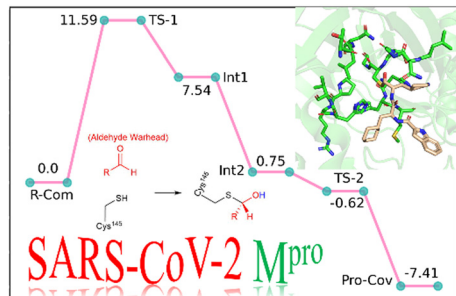
26298



One-pot self-assembled bimetallic sulfide particle cluster-supported three-dimensional graphene aerogel as an efficient electrocatalyst for the oxygen evolution reaction

Jianzhi Wang, Yu Luo, Jiwei Wang, Hongliang Yu, Ziyi Guo, Jie Yang, Yanan Xue, Ning Cai, Hui Li* and Faquan Yu*

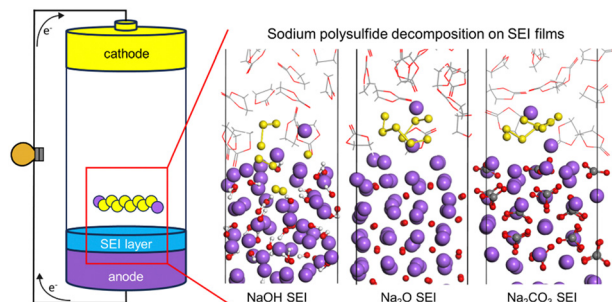
26308



Computational study on the mechanisms of inhibition of SARS-CoV-2 M^{pro} by aldehyde warheads based on DFT

Yongsheng Yang,* Chenghua Zhang, Xingcan Qian, Feiyan Jia and Shiwei Liang

26316



Role of inorganic layers on polysulfide decomposition at sodium-metal anode surfaces for room temperature Na/S batteries

Sirisak Singesen, Francisco Ospina-Acevedo, Suwit Suthirakun, Pussana Hirunsit and Perla B. Balbuena*

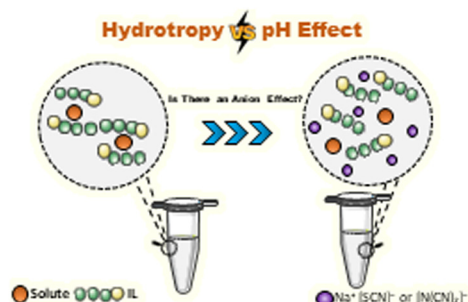


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26327

Exploring the impact of sodium salts on hydrotropic solubilization

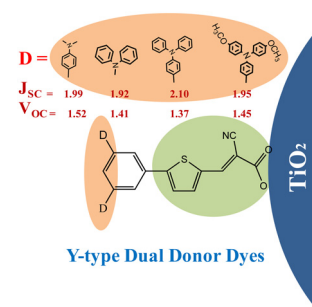
Jordana Benfica, Afonso C. Martins, Germán Pérez-Sánchez, Nicolas Schaeffer* and João A. P. Coutinho*



26341

A quantum chemical study: thoughtful exploration for optimal donors in Y-type dual donor-based dye sensitizers

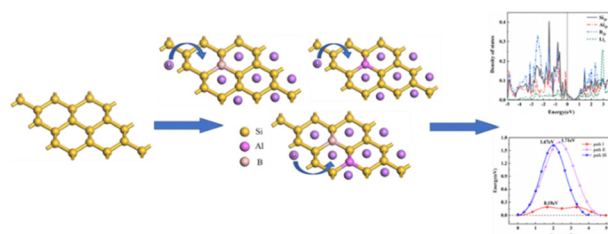
Anil Kumar Behera, Preeti Nanda Sahu, Ganesh Chandra Sahu and Anik Sen*



26353

Elucidating the effects of B/Al doping on the structure stability and electrochemical properties of silicene using DFT

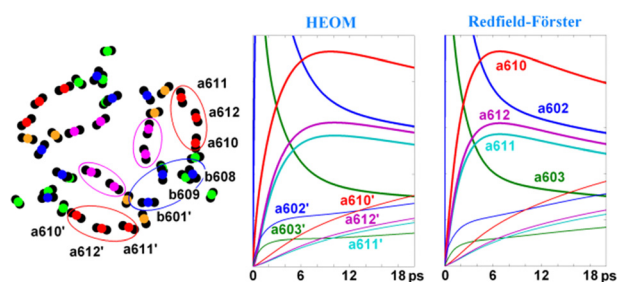
Ruyan Zhang, Yuhua Hou,* Xialei Guo, Xuan Chen, Wei Li, Xiaoma Tao and Youlin Huang*



26360

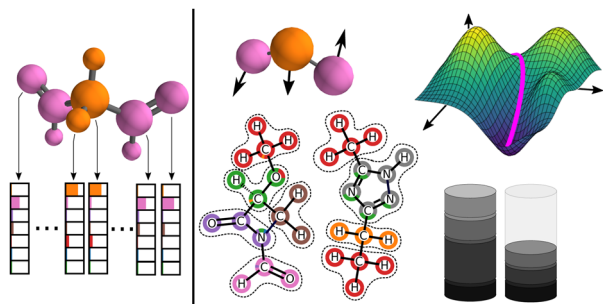
Excitation energy equilibration in a trimeric LHCII complex involves unusual pathways

Vladimir I. Novoderezhkin



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26370



Automatic identification of chemical moieties

Jonas Lederer,* Michael Gastegger, Kristof T. Schütt, Michael Kampffmeyer, Klaus-Robert Müller and Oliver T. Unke*

26380

Exact factorization based MQC methods					
COUPLED TRAJECTORIES			INDEPENDENT TRAJECTORIES		
Method	Nuclear Force	Quantum Momentum	Method	Nuclear Force	Quantum Momentum
CTMQC	EH + XF	Q_0 Q_m	MQC-XF	EH + XF	Q_0
CTSH	SH	Q_0 Q_m	SHXF	SH	Q_0
CTEh	EH	Q_0 Q_m	EhXF	EH	Q_0

Different flavors of exact-factorization-based mixed quantum-classical methods for multistate dynamics

Evaristo Villaseco Arribas, Patricia Vindel-Zandbergen, Saswata Roy and Neepta T. Maitra*

CORRECTION

26396

Correction: New insights into the 1D carbon chain through the RPA

Benjamin Ramberger and Georg Kresse*

