

IN THIS ISSUE

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Cover

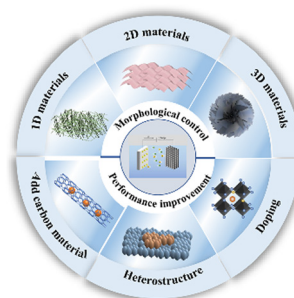
See Barbora Sedmidubská and Jaroslav Kočíšek, pp. 9112–9136. Image reproduced by permission of Barbora Sedmidubská and Jaroslav Kočíšek from *Phys. Chem. Chem. Phys.*, 2024, 26, 9112.

REVIEW

9096

Morphological control and performance engineering of Co-based materials for supercapacitors

Lin Pan, Dan Wang,* Jibiao Wang, Yuan Chu, Xiaosong Li, Wenchang Wang, Naotoshi Mitsuzaki, Shuyong Jia and Zhidong Chen*



PERSPECTIVES

9112

Interaction of low-energy electrons with radiosensitizers

Barbora Sedmidubská and Jaroslav Kočíšek*



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Fundamental questions
Elemental answers

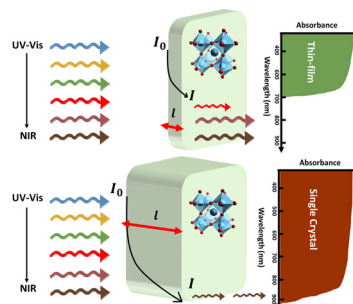


PERSPECTIVES

9137

Can thick metal-halide perovskite single crystals have narrower optical bandgaps with near-infrared absorption?

Mehri Ghasemi, Qianwen Wei, Junlin Lu, Yu Yang, Jingwei Hou, Baohua Jia* and Xiaoming Wen*

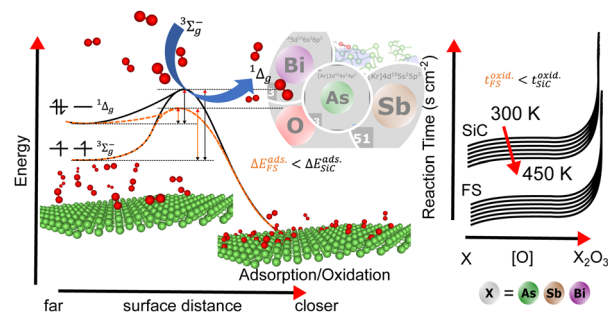


RESEARCH PAPERS

9149

Substrate suppression of oxidation process in pnictogen monolayers

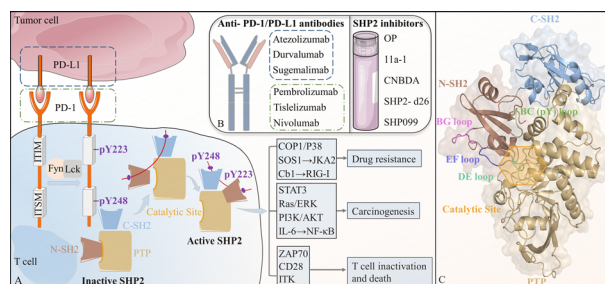
Rafael L. H. Freire, F. Crasto de Lima* and A. Fazzio



9155

Molecular recognition of ITIM/ITSM domains with SHP2 and their allosteric effect

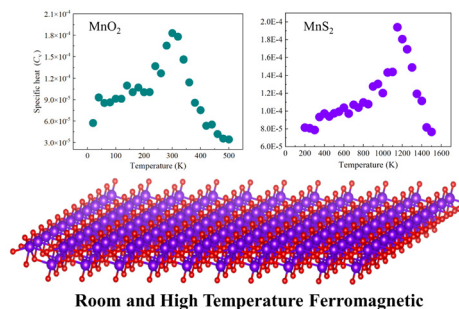
Yan Cheng, Weiwei Ouyang, Ling Liu, Ling kai Tang, Zhigang Zhang, Xinru Yue, Li Liang, Jianping Hu and Ting Luo*



9170

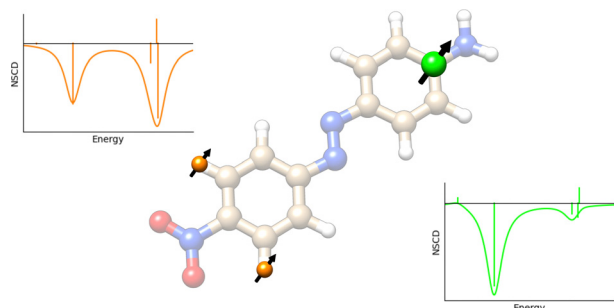
First-principles predictions of room-temperature ferromagnetism in orthorhombic MnX_2 ($\text{X} = \text{O}, \text{S}$) monolayers

Xuli Cheng, Shaowen Xu,* Tao Hu, Shunbo Hu,* Heng Gao, David J. Singh and Wei Ren*



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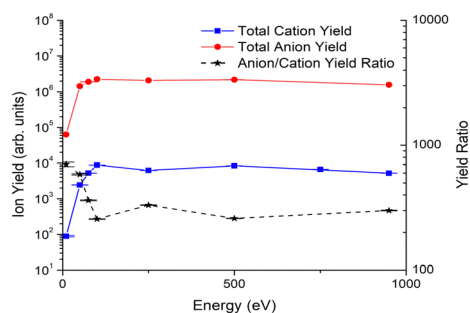
9179



Insights into localization, energy ordering, and substituent effect in excited states of azobenzenes from coupled cluster calculations of nuclear spin-induced circular dichroism

Josefine H. Andersen, Christof Hättig, Sonia Coriani* and Petr Štěpánek*

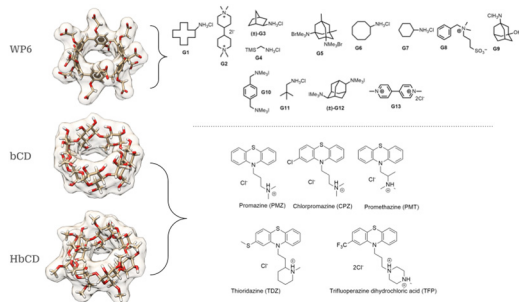
9197



Electron stimulated desorption from condensed benzene

L. Álvarez, A. D. Bass, A. I. Lozano, A. García-Abenza, P. Limão-Vieira, L. Sanche and G. García*

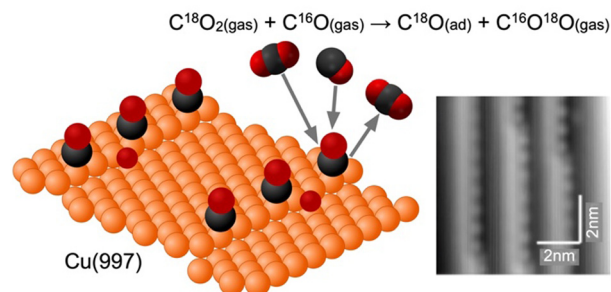
9207



The SAMPL9 host-guest blind challenge: an overview of binding free energy predictive accuracy

Martin Amezcua, Jeffry Setiadi and David L. Mobley*

9226



Low-temperature dissociation of CO₂ molecules on vicinal Cu surfaces

Takanori Koitaya,* Yuichiro Shiozawa, Yuki Yoshikura, Kozo Mukai, Shinya Yoshimoto and Jun Yoshinobu*

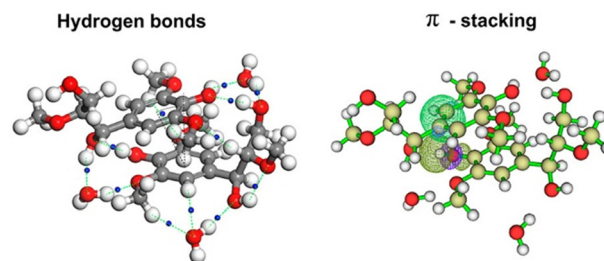


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9234

A density functional theory study on interactions in water-bridged dimeric complexes of lignin

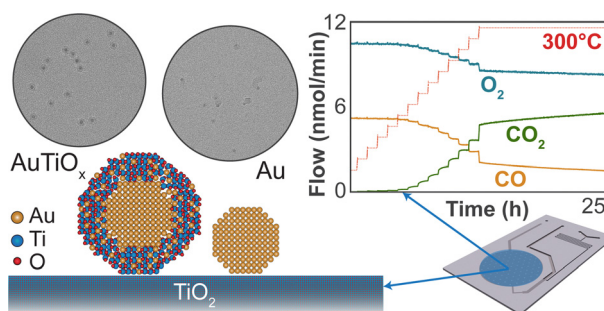
Jurgen Lange Bregado,* Argimiro R. Secchi and Frederico W. Tavares



9253

Stable mass-selected AuTiO_x nanoparticles for CO oxidation

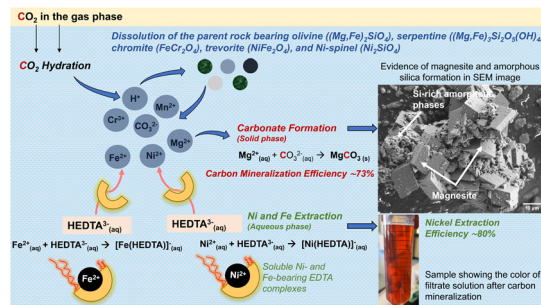
Rikke Egeberg Tankard, Filippo Romeggio, Stefan Kei Akazawa, Alexander Krabbe, Olivia Fjord Sloth, Niklas Mørch Secher, Sofie Colding-Fagerholt, Stig Helveg, Richard Palmer, Christian Danvad Damsgaard, Jakob Kibsgaard and Ib Chorkendorff*



9264

Mechanistic insights into the co-recovery of nickel and iron via integrated carbon mineralization of serpentinized peridotite by harnessing organic ligands

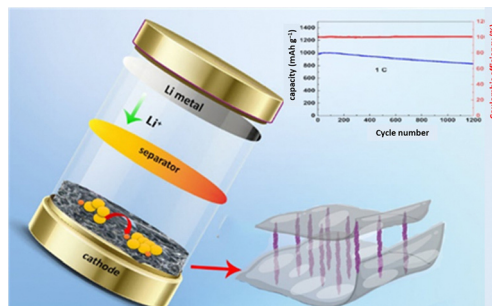
Shreya Katre, Prince Ochonma, Hassnain Asgar, Archana M Nair, Ravi K and Greeshma Gadikota*



9284

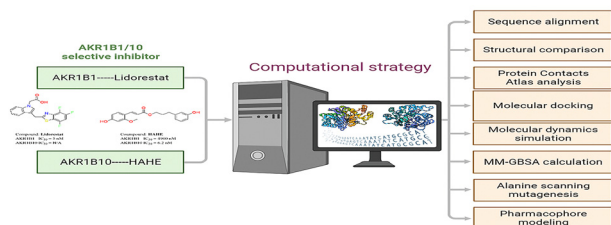
Vertical growth of a 3D Ni–Co-LDH/N-doped graphene aerogel: a cost-effective and high-performance sulfur host for Li–S batteries

Khalida Abaid Samawi, Bassam A. Mohammed, Ekhlas Abd-Alkuder Salman, HassabAlla M. A. Mahmoud, Aws Zuhair Sameen, Sura Mohammad Mohealdein, G. Abdulkareem-Alsultan* and Maadh Fawzi Nassar*



9295

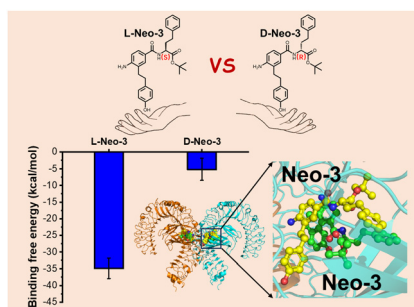
Decoding Selectivity: Computational Insights into AKR1B1 and AKR1B10 Inhibition



Decoding selectivity: computational insights into AKR1B1 and AKR1B10 inhibition

Mingyue Liu, Xiaochun Qin, Jing Li, Yuting Jiang, Junjie Jiang, Jiwei Guo, Hao Xu, Yousen Wang, Hengtai Bi and Zhiliang Wang*

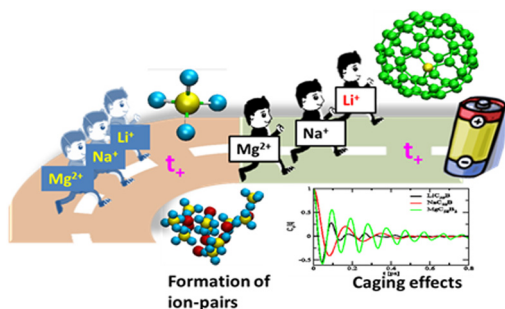
9309



Dissecting the chiral recognition of TLR4/MD2 with Neoseptin-3 enantiomers by molecular dynamics simulations

Cong Zhang, Siru Wu, Mingqi Li, Penghui Li, Xiubo Du, Yibo Wang* and Xiaohui Wang*

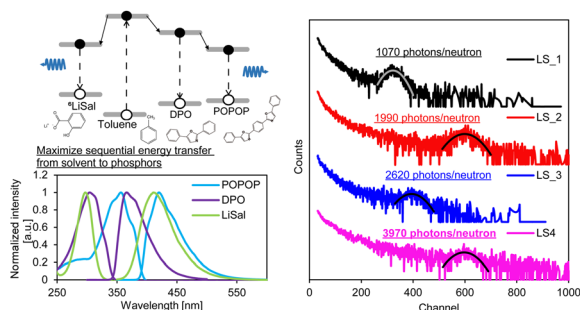
9317



Boron-containing fullerene-based salts with cyclic carbonate solvents as electrolytes for Li-ion batteries and beyond

Piyusaranjan Giri, Sourab Barath V., Shakuntala Dhurua, Sankar Maity, Rabiul Gazi and Madhurima Jana*

9329



Scintillation properties of lithium-6 salicylate-loaded liquid scintillators

Akito Watanabe,* Masanori Koshimizu,* Kenichi Watanabe, Atsushi Sato, Yutaka Fujimoto and Keisuke Asai

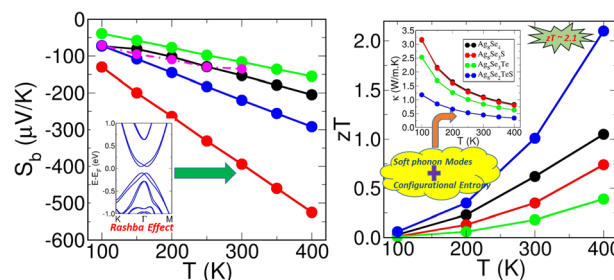


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9340

Computational approach to enhance thermoelectric performance of Ag_2Se by S and Te substitutions

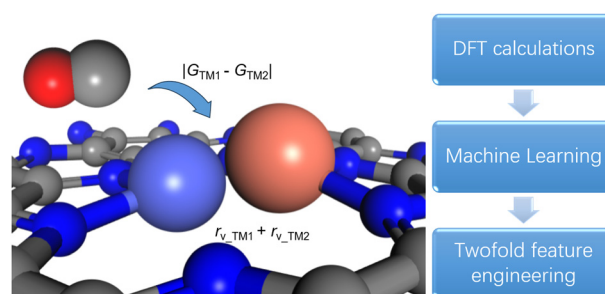
Raju K Biswas* and Swapan K Pati*



9350

Influence factors of CO adsorption on C_2N -supported dual-atom catalysts unveiled by machine learning and twofold feature engineering

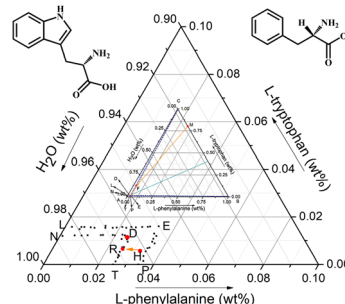
Shikai Chang, Hongshuai Wang, Yujin Ji* and Youyong Li*



9356

Study on the solid–liquid equilibrium and thermodynamic model of the L-phenylalanine + L-tryptophan + water system

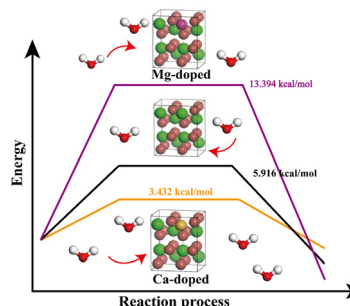
Weiping Liu, Hongfei Xiang, Yisong Wang, Xia Li, Yahui Yin, Yu Zhou and Xianzhen Xu*



9369

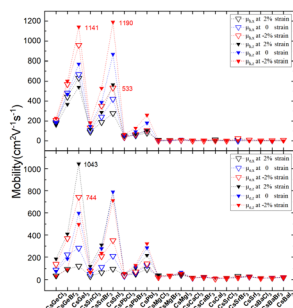
Adsorption behavior of H_2O on the strontium bromide surface: first-principles and molecular dynamics calculations

Zhen Wang, Ting Yan* and W. G. Pan*



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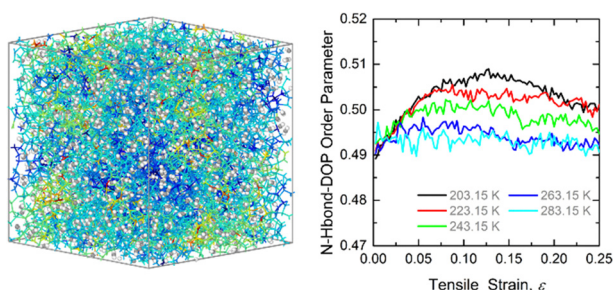
9378



High-throughput screening of the transport behavior of tetragonal perovskites

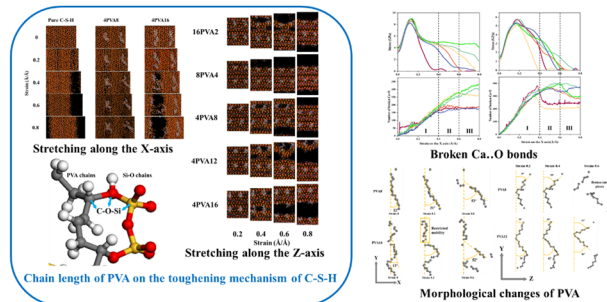
Yuanyuan Chen, Lu Xiao, Libin Shi* and Ping Qian*

9388

Mechanical properties of amorphous CO₂ hydrates: insights from molecular simulations

Pinqiang Cao,* Jianyang Wu and Fulong Ning

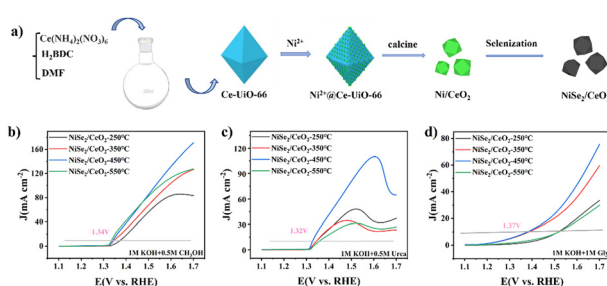
9399



The influence of the molecular chain length of PVA on the toughening mechanism of calcium silicate hydrates

Luqing Cheng, Yang Zhou,* Hao Zhang,* Shuai Xiao, Weihuan Li and Wentao Chen

9413

NiSe₂/CeO₂ catalysts from Ce-Uio-66 metal-organic skeletons and their electrocatalytic oxidation of methanol, urea and glycerol

Jiaqi Huo, Ying Chang,* Aiju Xu, Meilin Jia and Jingchun Jia*

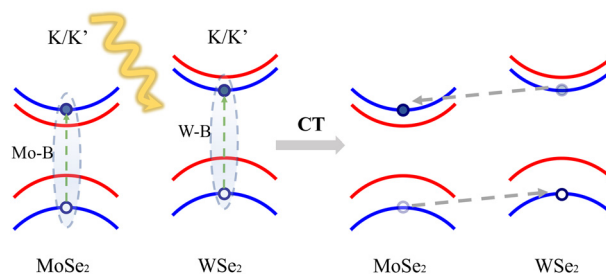


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9424

A new charge transfer pathway in the MoSe₂–WSe₂ heterostructure under the conditions of B-excitons being resonantly pumped

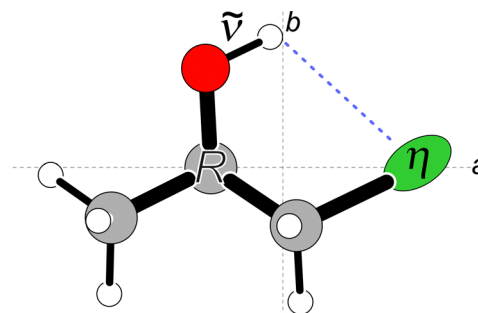
Zifan Hu, Hai Wang, Lei Wang and Haiyu Wang*



9432

Weak hydrogen bonding to halogens and chirality communication in propanols: Raman and microwave spectroscopy benchmark theory

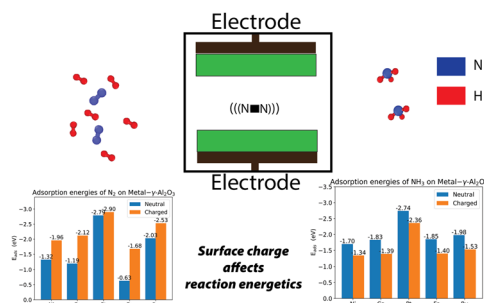
Beppo Hartwig, Melanie Schnell, Martin A. Suhm and Daniel A. Obenchain*



9453

Modelling the effect of surface charging on plasma synthesis of ammonia using DFT

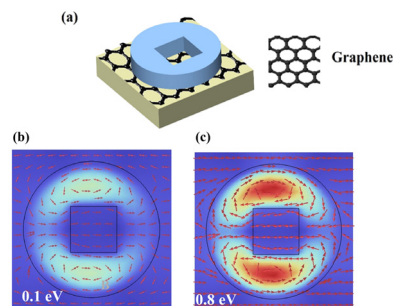
Aditya Dilip Lele,* Yijie Xu and Yiguang Ju



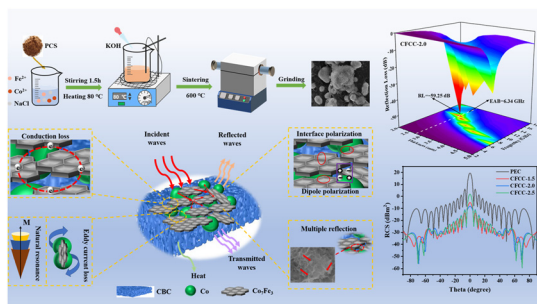
9462

A triple Fano resonance Si-graphene metasurface for multi-channel tunable ultra-narrow band sensing

Jukun Liu,* Hongxiang Dai, Jiaqi Ju* and Ke Cheng



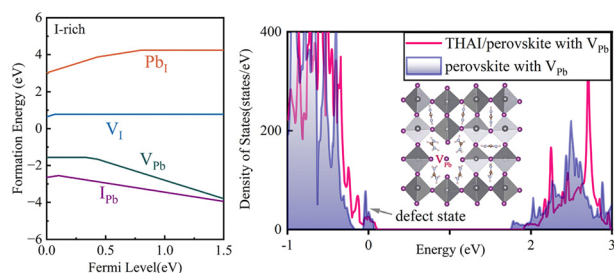
9475



One-step sintering construction of electromagnetic synergistic $\text{Co}_7\text{Fe}_3/\text{Co}@\text{CBC}$ nanocomposites for enhanced microwave absorption properties

Yunmin Zhao, Shunlin Su, Zhilong Liu, Jianxin Ren, Lihong Wang* and Yude Wang*

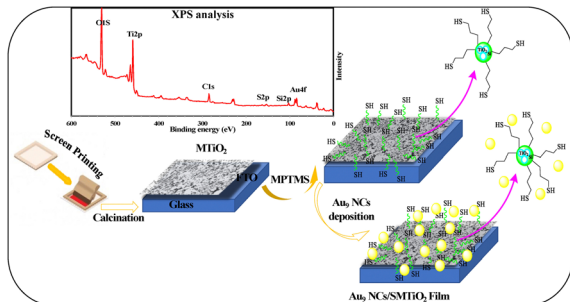
9488



Rational control of the typical surface defects of hybrid perovskite using tetrahexylammonium iodide

Ben Wang, Shunwei Yao, Wenjing Hu, Lin Peng,* Tingting Shi, Yanan Wang, Jing Chen, Xiaolin Liu and Jia Lin*

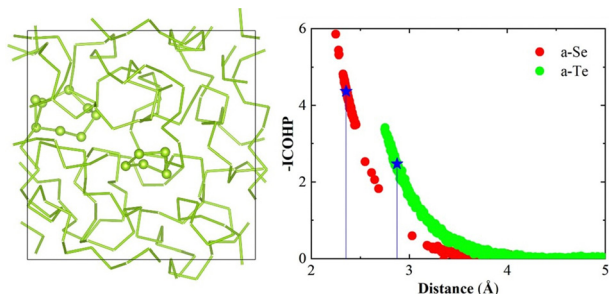
9500



Au_9 nanocluster adsorption and agglomeration control through sulfur modification of mesoporous TiO_2

Anahita Motamedisade, Martin R. Johnston, Amjad E.H. Alotaibi and Gunther A. Andersson*

9510



Structure, bonding and electronic characteristics of amorphous Se

Chong Qiao, Lanli Chen, Rongchuan Gu, Bin Liu, Shengzhao Wang, Songyou Wang, Cai-Zhuang Wang, Kai-Ming Ho, Ming Xu* and Xiangshui Miao

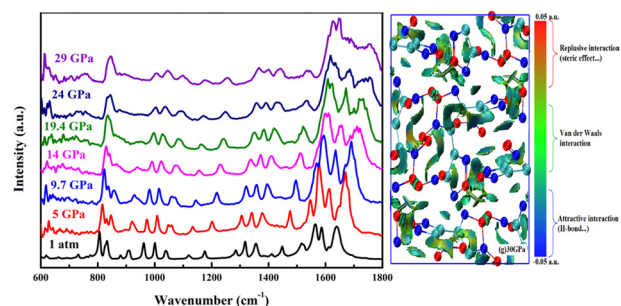


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9517

Infrared spectra and electronic structural changes of DNTF under high pressure: experimental and theoretical studies

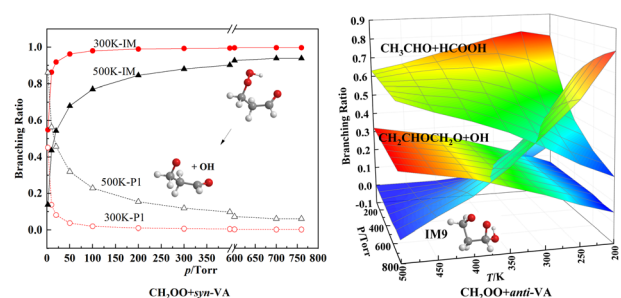
Hai Nan, Haipeng Su, Chunyan Chen, Yufan Bu, Guotao Niu, Peipei Sun, Fei Shen and Xuanjun Wang*



9524

Pressure and temperature dependent kinetics and the reaction mechanism of Criegee intermediates with vinyl alcohol: a theoretical study

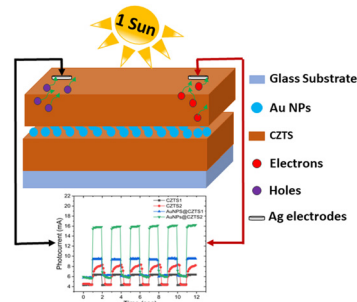
Cuihong Sun, Baoen Xu and Yanli Zeng*



9534

Microstrain effects of laser-ablated Au nanoparticles in enhancing CZTS-based 1 Sun photodetector devices

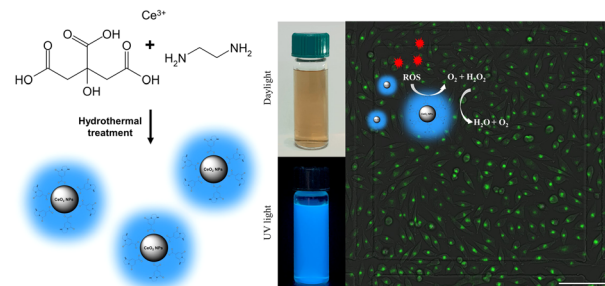
Serap Yiğit Gezgin, Walid Belaid, Mohamed A. Basyooni-M. Kabatas,* Yasin Ramazan Eker and Hamdi Şükür Kilic



9546

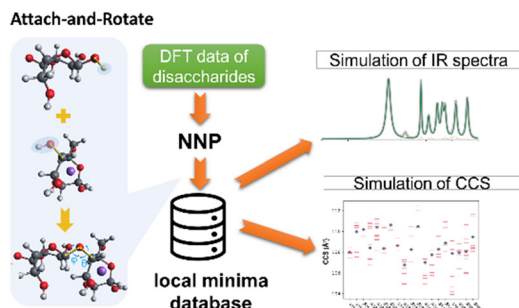
One-pot hydrothermal synthesis of fluorophore-modified cerium oxide nanoparticles

Daria V. Tsyupka,* Sergey V. Pigarev, Yuliya A. Podkolodnaya, Ekaterina A. Khudina, Nelli R. Popova, Irina Yu. Goryacheva and Olga A. Goryacheva



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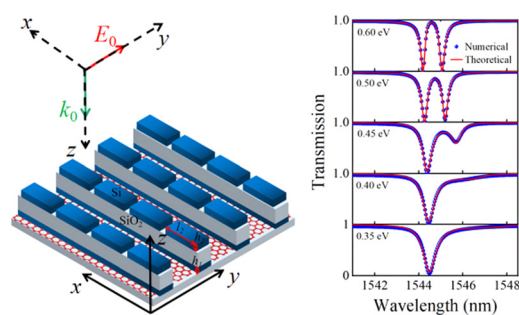
9556



A first-principles exploration of the conformational space of sodiated di-saccharides assisted by semi-empirical methods and neural network potentials

Huu Trong Phan, Pei-Kang Tsou, Po-Jen Hsu and Jer-Lai Kuo*

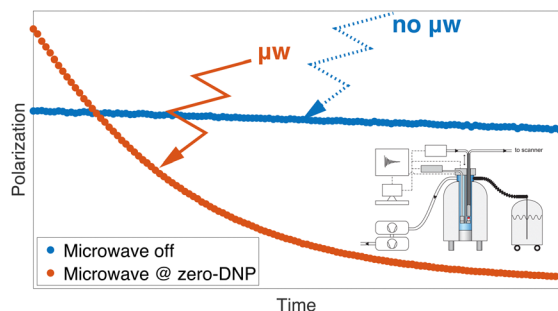
9568



Active control of an electromagnetically induced transparency analogue in a coupled dual bound states in the continuum system integrated with graphene

Fan Jiang, Yanxin Lu and Yihang Chen*

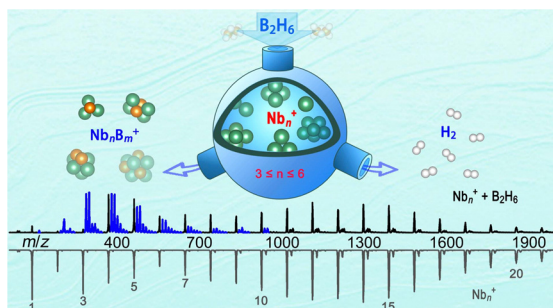
9578



Relaxation enhancement by microwave irradiation may limit dynamic nuclear polarization

Gevin von Witte, Aaron Himmler, Sebastian Kozerke and Matthias Ernst*

9586



Dehydrogenation of diborane on small Nb_n^+ clusters

Wen Gan, Lijun Geng, Benben Huang, Klavs Hansen and Zhixun Luo*

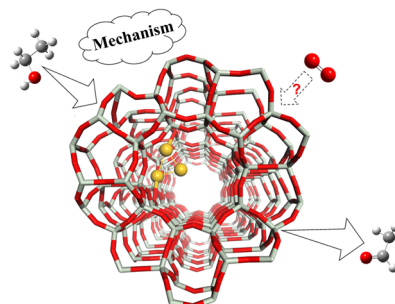


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9593

Computational insights into the zeolite-supported gold nanocluster-catalyzed ethanol dehydrogenation to acetaldehyde

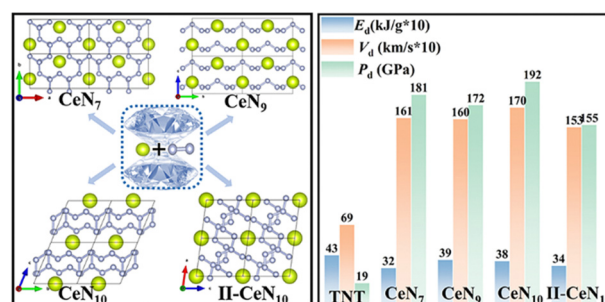
Yi Zhang, Kangjian Tang* and Xiaoguang Bao*



9601

Nitrogen-rich Ce–N compounds under high pressure

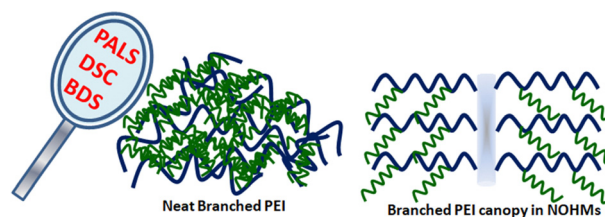
Yuan-Yuan Wang, Shuang Liu, Shuang-Chen Lu,* Yi Li and Zhen Yao*



9608

Interfacial-interaction induced modifications in segmental dynamics and free volume of the poly(ethyleneimine) canopy in nanoparticle–organic hybrid materials: an investigation by temperature dependent broadband dielectric and positron annihilation spectroscopy

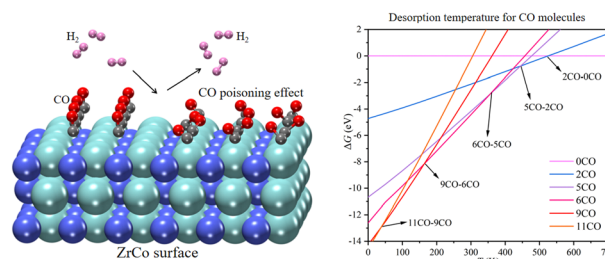
Jaideep Mor, Renjith B. Nelliyl and Sandeep Kumar Sharma*



9617

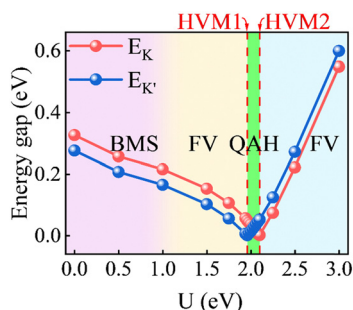
Unraveling CO adsorption behaviors and its poisoning effects on ZrCo surface

Yuejing Lan, Ru Tang, Rongxing Ye, Minan Su, Qianghua Lei, Fei Li,* Xiaofeng Tian, Jiangfeng Song and Linsen Zhou*



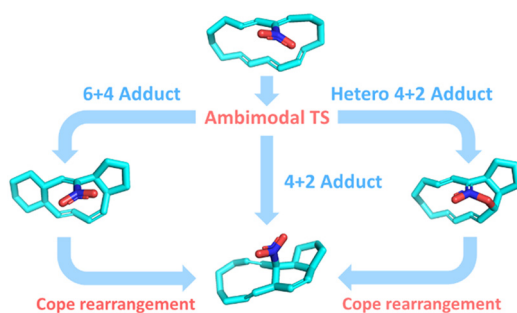
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9628

Influence of electronic correlation on the valley and topological properties of VSiGeP₄ monolayer

Guangxin Fan, Yanzhao Wu, Junwei Tong, Li Deng, Xiang Yin, Fubo Tian and Xianmin Zhang*

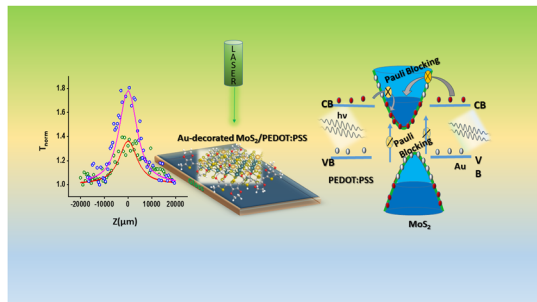
9636



Substituent effects on the selectivity of ambimodal [6+4]/[4+2] cycloaddition

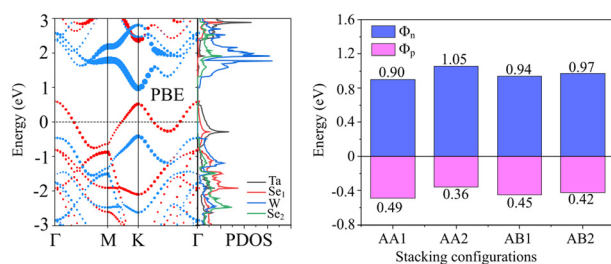
Wenhao Gu and John Z.H. Zhang*

9645

Enhancing saturable absorption in a Au-decorated MoS₂/PEDOT:PSS nanocomposite through plasmon resonance and Pauli blocking

Arjun K., Amaljith C. K. and Karthikeyan B.*

9657

Controllable electronic properties, contact barriers and contact types in a TaSe₂/WSe₂ metal–semiconductor heterostructure

Son T. Nguyen, Nguyen Cuong Q.,* Nguyen N. Hieu, H. V. Phuc* and Ch. V. Nguyen

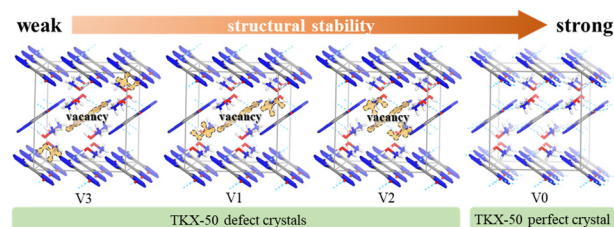


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9665

Structural and decomposition analysis of TKX-50 with vacancy defects: insights from DFT and AIMD simulations

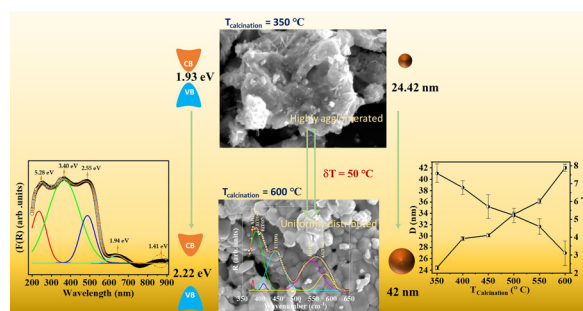
Zhiwei Guo, Xiaohe Wang, Gazi Hao, Lei Xiao, Xiaojun Feng, Junqing Yang* and Wei Jiang*



9675

Interband electronic transitions and optical phonon modes in size-dependent multiferroic BiFeO₃ nanoparticles

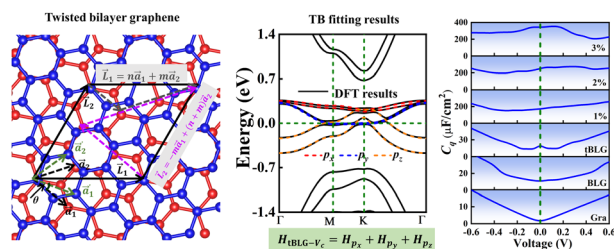
Priyambada Sahoo and Ambesh Dixit*



9687

Electronic structures and quantum capacitance of twisted bilayer graphene with defects based on three-band tight-binding model

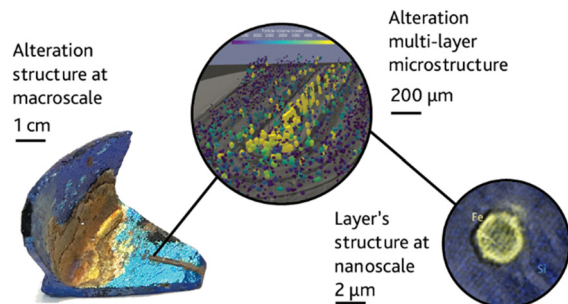
Baojuan Xin, Kaixin Zou, Dayong Liu, Boyan Li, Hong Dong, Yahui Cheng, Hui Liu, Liang-Jian Zou, Feng Luo, Feng Lu* and Wei-Hua Wang*



9697

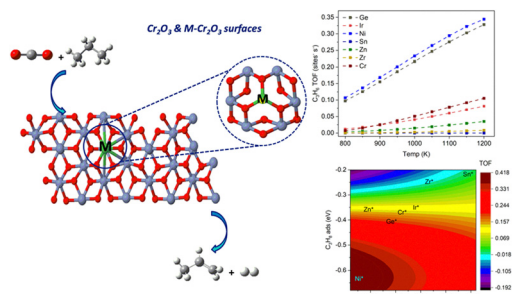
Non-destructive 3D exploration of silicate glass corrosion: a combined multiscale approach from the macro to the nanoscale

Giulia Franceschin*, Roberta Zanini, Gianluca Iori, Elena Longo, Giorgio Divitini, Giuliana Tromba and Arianna Travaglia



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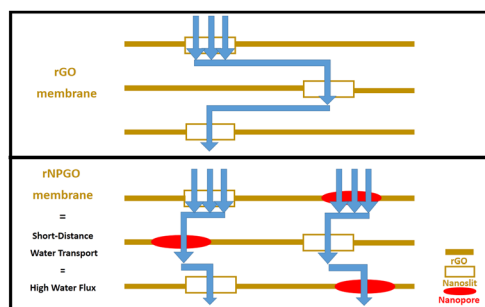
9708



Enhancing catalytic activity of Cr_2O_3 in CO_2 -assisted propane dehydrogenation with effective dopant engineering: a DFT-based microkinetic simulation

Faheem Jan, Shuaike Zhi, XiaoYing Sun* and Bo Li*

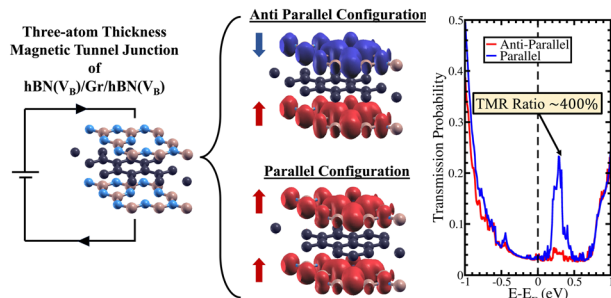
9722



Enhancing the seawater desalination performance of multilayer reduced graphene oxide membranes by introducing in-plane nanopores: a molecular dynamics simulation study

Z. Alinia, H. Akbarzadeh,* F. Mohammadi Zonoz and R. Tayebee

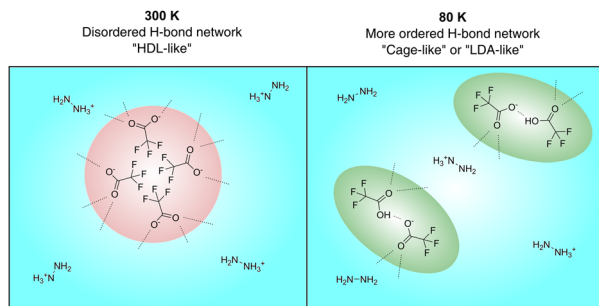
9733



Ultra-thin van der Waals magnetic tunnel junction based on monoatomic boron vacancy of hexagonal boron nitride

Halimah Harfah,* Yusuf Wicaksono, Gagus Ketut Sunnardianto, Muhammad Aziz Majidi and Koichi Kusakabe

9741



Tuning the low-temperature phase behavior of aqueous ionic liquids

Johannes Bachler, Isabella Daidone, Laura Zanetti-Polzi and Thomas Loerting*



9754

A novel method of alkoxyamine homolysis activation *via* photochemical rearrangement

Sergey Cherkasov,* Dmitriy Parkhomenko,
Denis Morozov and Elena Bagryanskaya

