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See Yoonsoo Pang *et al.*, pp. 11283–11294. Image reproduced by permission of Yoonsoo Pang from *Phys. Chem. Chem. Phys.*, 2024, 26, 11283.



Inside cover

See Enrique M. Arpa, Bo Durbéej *et al.*, pp. 11295–11305. Image reproduced by permission of Enrique Manuel Arpa and Bo Durbéej from *Phys. Chem. Chem. Phys.*, 2024, 26, 11295.

TUTORIAL REVIEW

11182

A comprehensive review of oxygen vacancy modified photocatalysts: synthesis, characterization, and applications

Faqi Zhan,* Guochang Wen, Ruixin Li, Chenchen Feng, Yisi Liu, Yang Liu, Min Zhu, Yuehong Zheng, Yanchun Zhao* and Peiqing La*

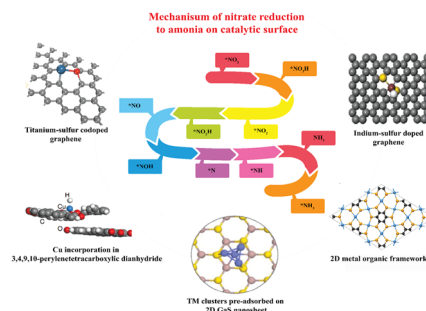


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Recent progress in the advanced strategies, rational design, and engineering of electrocatalysts for nitrate reduction toward ammonia

Faiza Shafiq, Lei Yang and Weihua Zhu*



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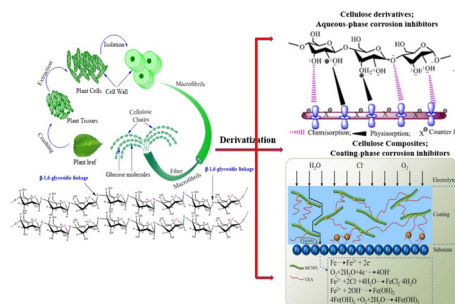
Fundamental questions
Elemental answers

REVIEWS

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Cellulose, cellulose derivatives and cellulose composites in sustainable corrosion protection: challenges and opportunities

Chandrabhan Verma,* Vidusha Singh and Akram AlFantazi*

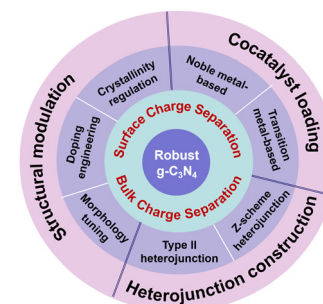


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Progress on enhancing the charge separation efficiency of carbon nitride for robust photocatalytic H₂ production

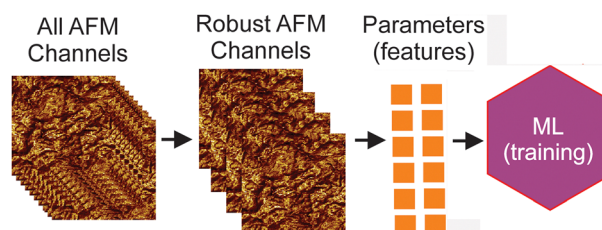
Mengmeng Shao,* Yangfan Shao and Hui Pan*



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On machine learning analysis of atomic force microscopy images for image classification, sample surface recognition

I. Sokolov

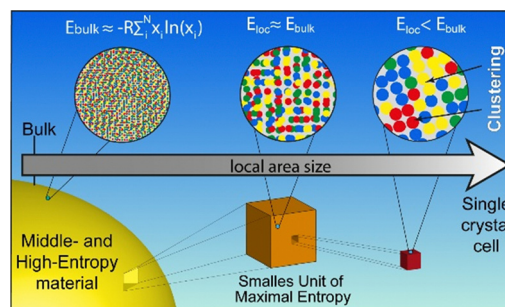


COMMUNICATIONS

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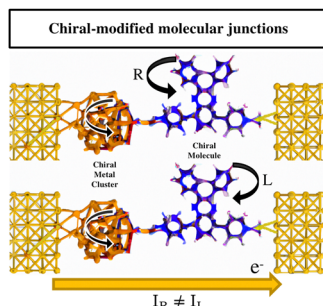
Smallest unit of maximal entropy as novel experimental criterion for parametric characterization of middle- and high-entropy materials

Alexander Khort,* Alexander Dahlström, Sergey Roslyakov and Inger Odneval



COMMUNICATIONS

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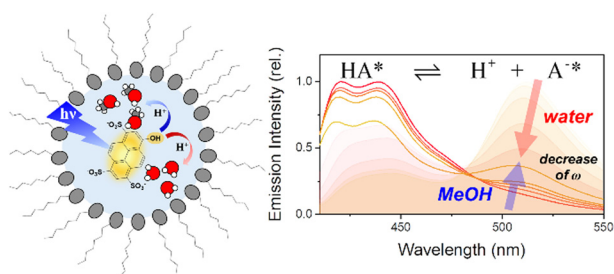


A chiral metal cluster triggers enantiospecific electronic transport

Omar Hernández-Montes, Ignacio L. Garzón and J. Eduardo Barrios-Vargas*

RESEARCH PAPERS

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Anomalous proton transfer of a photoacid HPTS in nonaqueous reverse micelles

Taehyung Jang, Sebok Lee and Yoonsoo Pang*

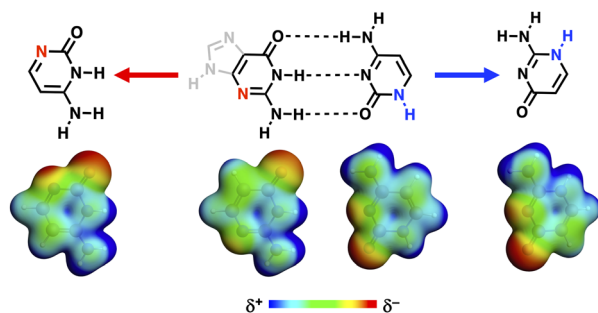
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Photochemical formation of the elusive Dewar isomers of aromatic systems: why are substituted azaborines different?

Enrique M. Arpa,* Sven Stafström and Bo Durbeej*

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Multiple hydrogen-bonded dimers: are only the frontier atoms relevant?

Celine Nieuwland, David Almacellas, Mac M. Veldhuizen, Lucas de Azevedo Santos, Jordi Poater and Célia Fonseca Guerra*

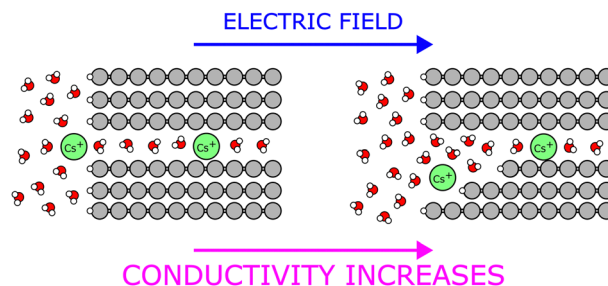


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Cs⁺ conductance in graphene membranes with Ångström-scale pores: the role of pore entrance geometry

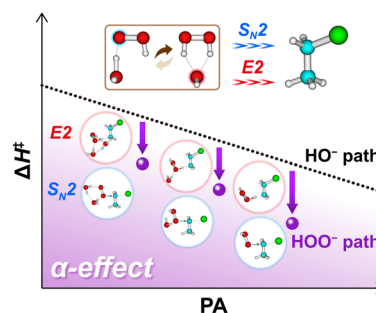
Enrique Wagemann, Na Young Kim and Sushanta K. Mitra*



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Solvent-induced dual nucleophiles and the α -effect in the S_N2 versus E2 competition

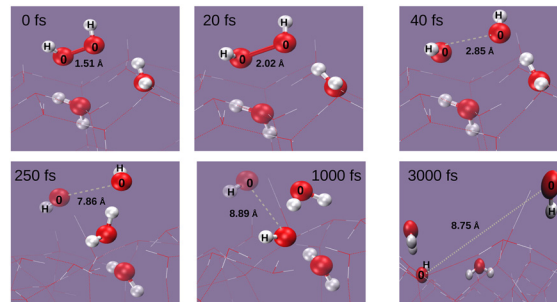
Xiangyu Wu, F. Matthias Bickelhaupt* and Jing Xie*



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Dissociation of H₂O₂ on water surfaces (ice and water droplets)

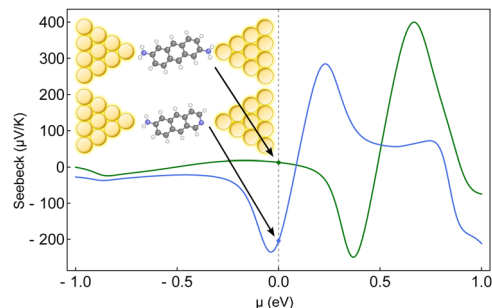
Amit Kumar and Pradeep Kumar*



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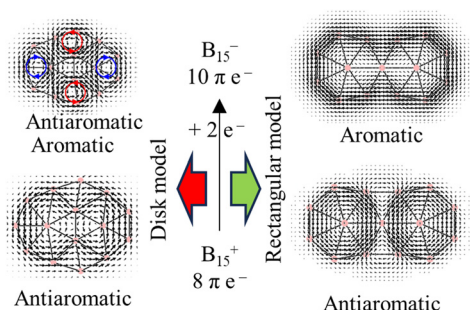
Enhancing the thermopower of single-molecule junctions by edge substitution effects

Qiang Qi, Guangjun Tian and Liang Ma*



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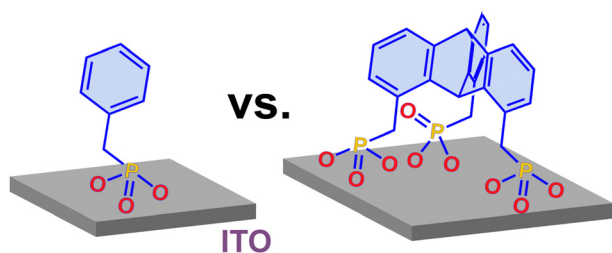
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A reinvestigation of the boron cluster $B_{15}^{+/-0}$: a benchmark of density functionals and consideration of aromaticity models

Yassin A. Jeilani, Long Van Duong,* Obaid Moraya Saeed Al Qahtani and Minh Tho Nguyen

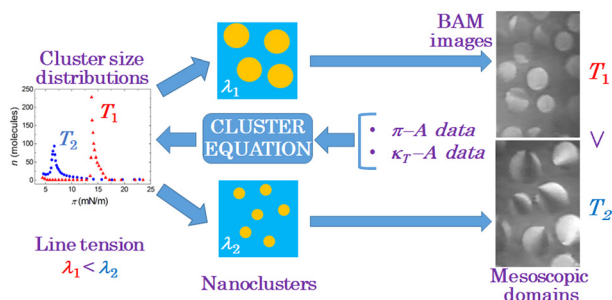
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Phosphonic acid anchored tripodal molecular films on indium tin oxide

Chaoran Zhang, Saunak Das, Naoya Sakurai, Takaki Imaizumi, Sajisha Sanjayan, Yoshiaki Shoji, Takanori Fukushima* and Michael Zharnikov*

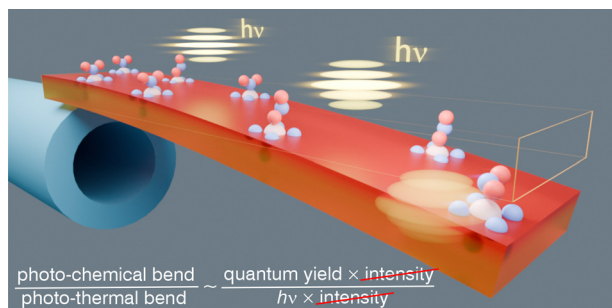
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Hierarchical structure growth across different length scales in the two-phase coexistence region of myristic acid Langmuir monolayers: correlation of static and dynamic heterogeneities

E. Hatta

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Determining the quantum yield of photochemical reactions in crystals from simultaneous effects of photothermal and photochemical bending of needle-shaped crystals

Stanislav Chizhik,* Pavel Gribov, Viktor Kovalskii and Anatoly Sidelnikov

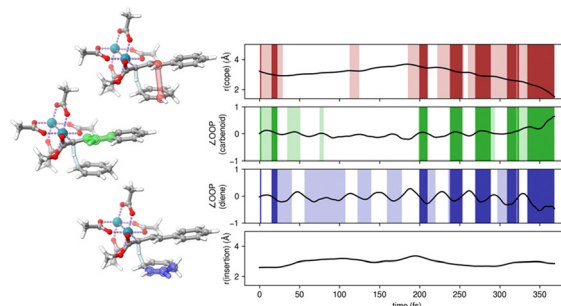


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Vibrational synchronization and its reaction pathway influence from an entropic intermediate in a dirhodium catalyzed allylic C–H activation/Cope rearrangement reaction

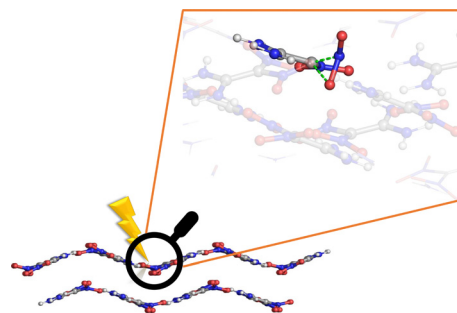
Anthony J. Schaefer and Daniel H. Ess*



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Initial decomposition pathways of 1,1-diamino-2,2-dinitroethylene (α -FOX-7) in the condensed phase

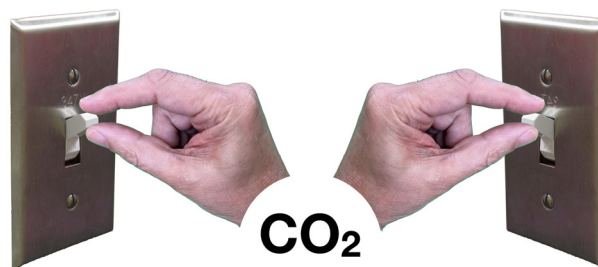
Komal Yadav, Yuheng Luo, Ralf I. Kaiser and Rui Sun*



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Simultaneous switching of two different CO₂-switchable amines in the same solution

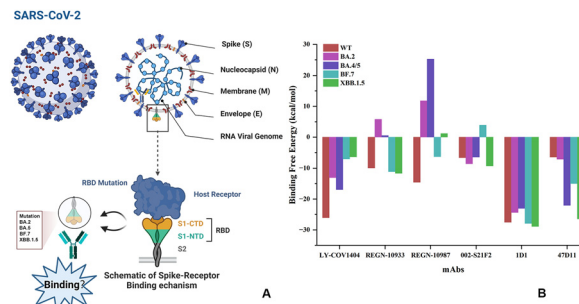
Matthew Sanger, Daniel Barker and Philip G. Jessop*



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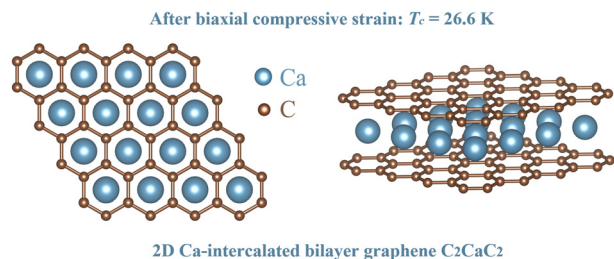
Evaluating mAbs binding abilities to Omicron subvariant RBDs: implications for selecting effective mAb therapies

Song Luo, Danyang Xiong, Bolin Tang, Bangyu Liu, Xiaoyu Zhao and Lili Duan*



RESEARCH PAPERS

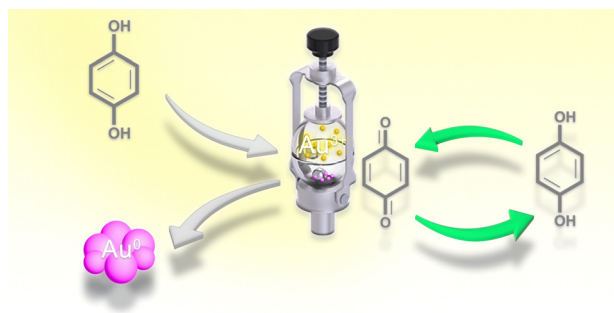
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Superconductivity in Ca-intercalated bilayer graphene: C_2CaC_2

Jin-Han Tan, Hao Wang, Ying-Jie Chen, Na Jiao, Meng-Meng Zheng,* Hong-Yan Lu* and Ping Zhang*

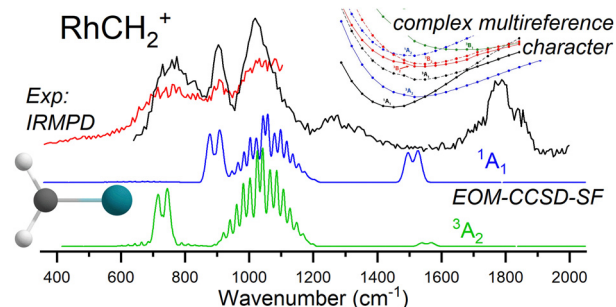
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Mechanochemical hydroquinone regeneration promotes gold salt reduction in sub-stoichiometric conditions of the reducing agent

Ismael P. L. Xavier, Laura L. Lemos, Eduardo C. de Melo, Eduardo T. Campos, Breno L. de Souza, Leandro A. Faustino, Douglas Galante and Paulo F. M. de Oliveira*

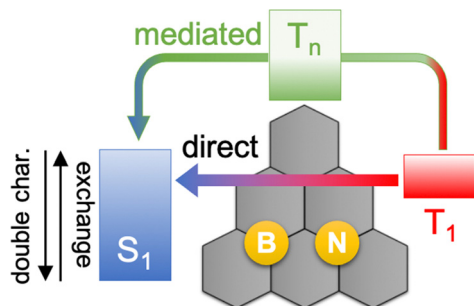
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IR spectroscopic characterization of $[M,C,2H]^+$ ($M = Ru$ and Rh) products formed by reacting 4d transition metal cations with oxirane: Spectroscopic evidence for multireference character in $RhCH_2^+$

Frank J. Wensink, Corry E. Smink, Brandon C. Stevenson, Ryan P. Steele, Joost M. Bakker* and P. B. Armentrout*

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Reverse intersystem crossing mechanisms in doped triangulenes

Asier E. Izu, Jon M. Matxain and David Casanova*

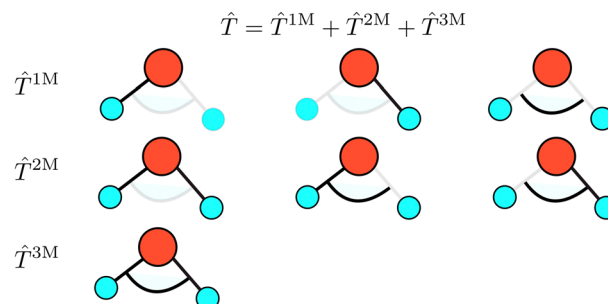


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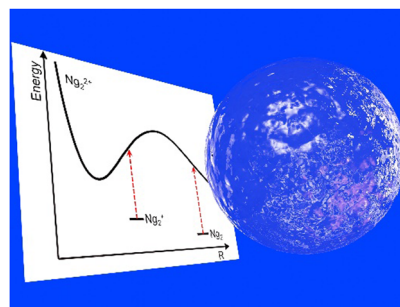
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Efficient vibrationally correlated calculations using n -mode expansion-based kinetic energy operators

Frederik Bader,* David Lauvergnat and Ove Christiansen



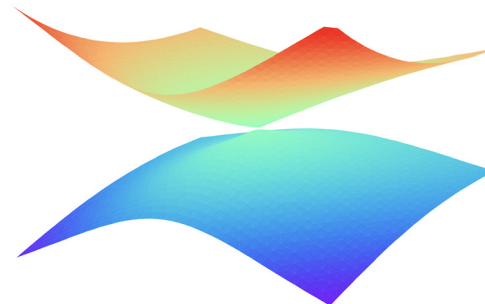
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Doubly charged dimers and trimers of heavy noble gasesGabriel Schöpfer, Stefan Bergmeister, Milan Ončák,*
Ianessa Stromberg, Masoomah Mahmoodi-Darian,
Paul Scheier, Olof Echt* and Elisabeth Gruber

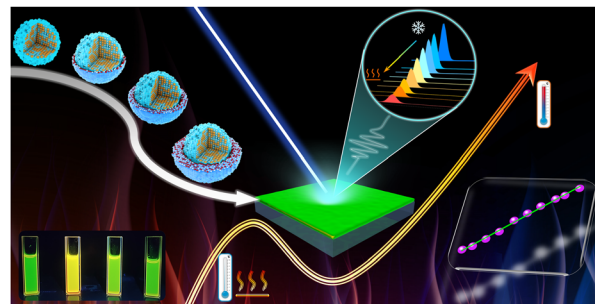
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Quantum simulation of conical intersections

Yuchen Wang and David A. Mazziotti*

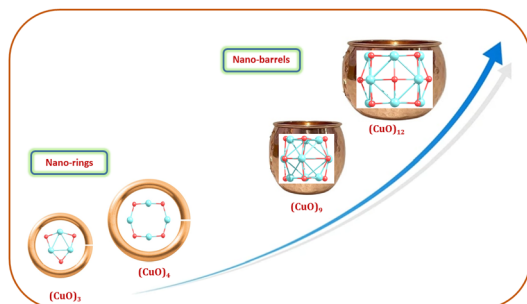


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Shell thickness-induced thermal dependence: highly sensitive core-shell CdSe/ZnS/POSS-based temperature probesJiannan Sun, Ke Yan,* Aizhao Pan,* Pan Zhang,*
Xuehang Chen, Xinyi Shi and Chengyu Shi

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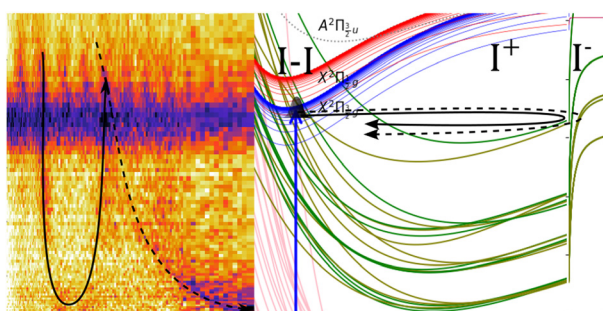
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Evolution of the atomic and electronic structures of CuO clusters: a comprehensive study using the DFT approach

Soumitra Das,* Sandeep Nigam, Pramod Sharma and Chiranjib Majumder*

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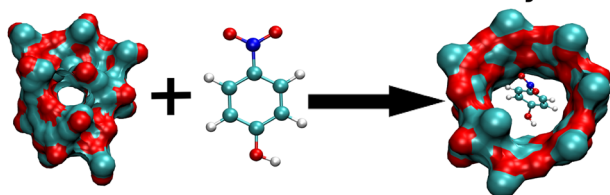


Real-time dynamics of vibronic wavepackets within Rydberg and ion-pair states of molecular iodine

Jean-Michel Mestdagh, Lou Barreau and Lionel Poisson*

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Substitution distorts CD cavity

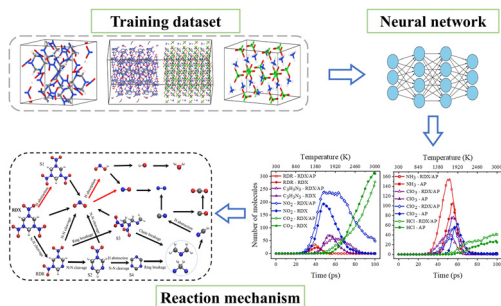


Inclusion of guest stabilizes the cavity

The counteracting influence of 2-hydroxypropyl substitution and the presence of a guest molecule on the shape and size of the β -cyclodextrin cavity

Avilasha A. Sandilya and M. Hamsa Priya*

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The thermal decomposition mechanism of RDX/AP composites: *ab initio* neural network MD simulations

Kehui Pang, Mingjie Wen, Xiaoya Chang, Yabei Xu, Qingzhao Chu* and Dongping Chen*

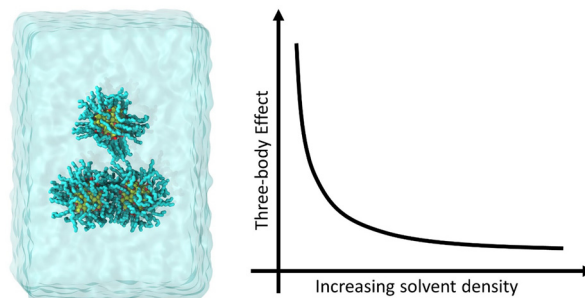


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Three-body interaction of gold nanoparticles: the role of solvent density and ligand shell orientation

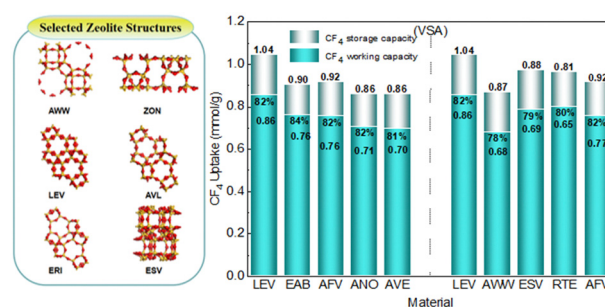
Hari O. S. Yadav



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High throughput screening of pure silica zeolites for CF₄ capture from electronics industry gas

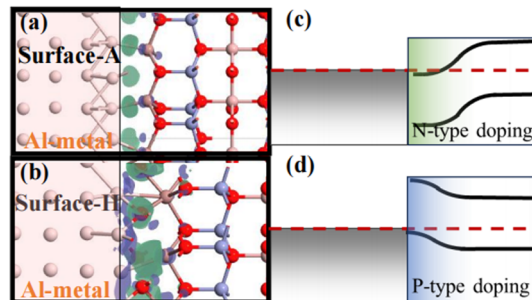
Hui-Dong Zhang, Xiao-Dong Li,* Yan-Yu Xie, Peng-Hui Yang and Jing-Xin Yu



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Physical insight of random fluctuation in metal/IGZO Schottky barriers for low-variation contact optimal design

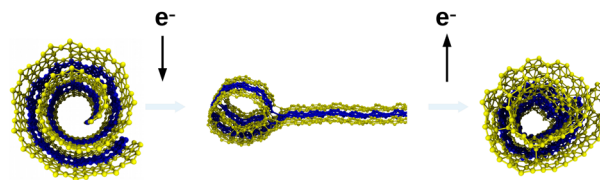
Lijun Xu, Kun Luo, Guohui Zhan, Jiangtao Liu and Zhenhua Wu*



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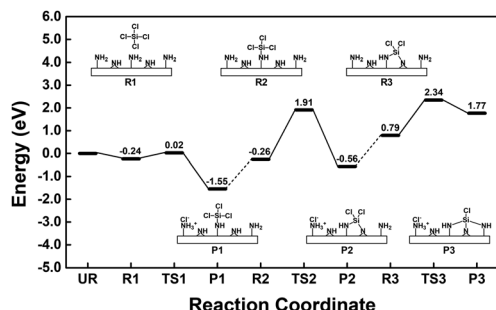
Reversible actuation of α -borophene nanoscrolls

Guilherme S. L. Fabris, Douglas S. Galvão* and Ricardo Paupitz*



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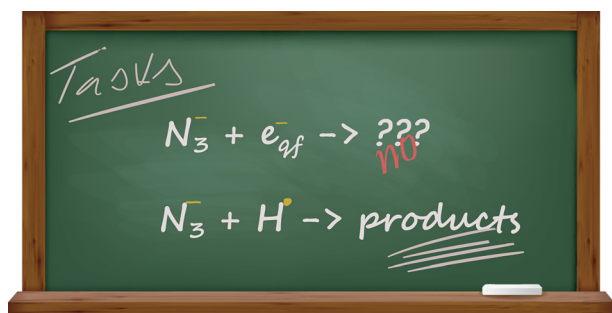
11597



Chemisorption of silicon tetrachloride on silicon nitride: a density functional theory study

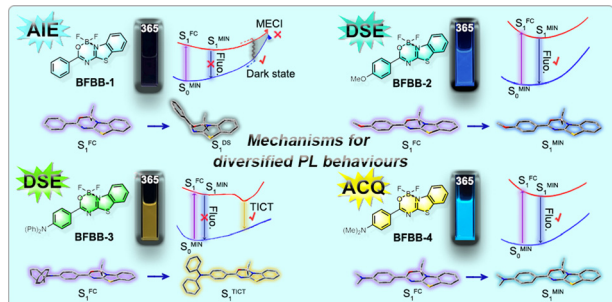
Tanzia Chowdhury, Khabib Khumaini, Romel Hidayat, Hye-Lee Kim and Won-Jun Lee*

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Reactivity of quasi-free electrons toward N_3^- and its impact on H_2 formation mechanism in water radiolysis

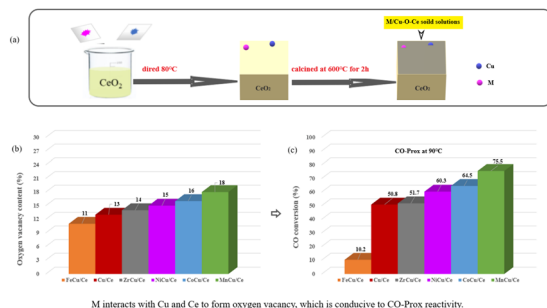
Denis Dobrovolskii, Sergey A. Denisov, Howard E. Sims and Mehran Mostafavi*

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Mechanistic insights into diversified photoluminescence behaviours of BF_2 complexes of *N*-benzoyl 2-aminobenzothiazoles

He Zheng, Yan-Xue Li, Wen-Chao Xiong, Xing-Cong Wang, Shan-Shan Gong, Shouzhi Pu,* Rongwei Shi* and Qi Sun*

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Different metal (Mn, Fe, Co, Ni, and Zr) decorated Cu/CeO₂ catalysts for efficient CO oxidation in a rich CO₂/H₂ atmosphere

Yue Xing, Jiaxin Wu, Daosheng Liu, Caishun Zhang, Jiao Han, Honghao Wang, Yinfu Li, Xiaoning Hou, Lei Zhang* and Zhixian Gao*

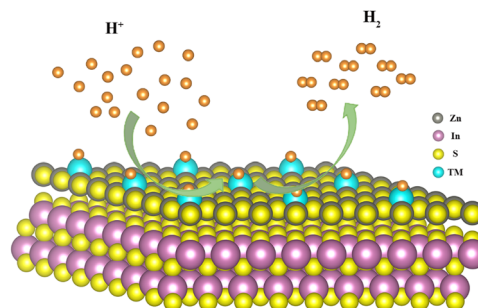


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Transition metal single-atoms supported on hexagonal ZnIn_2S_4 monolayers for the hydrogen evolution reaction

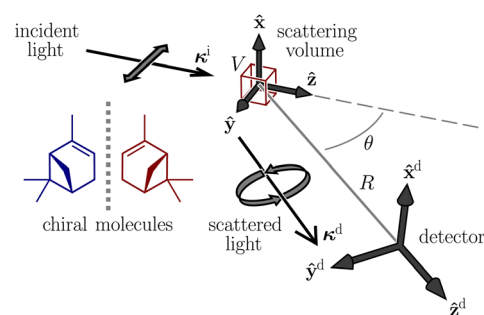
Xiujuan Cheng, Kunyang Cheng, Xuying Zhou, Mingyang Shi, Gang Jiang and Jiguang Du*



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Theory of Rayleigh–Brillouin optical activity light scattering applicable to chiral liquids

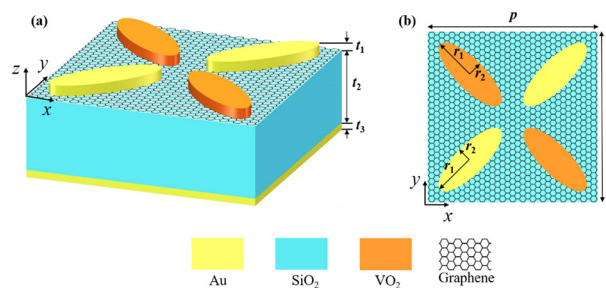
Robert P. Cameron,* Emmanouil I. Alexakis, Aidan S. Arnold and Duncan McArthur



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Actively tunable and switchable terahertz metamaterials with multi-band perfect absorption and polarization conversion

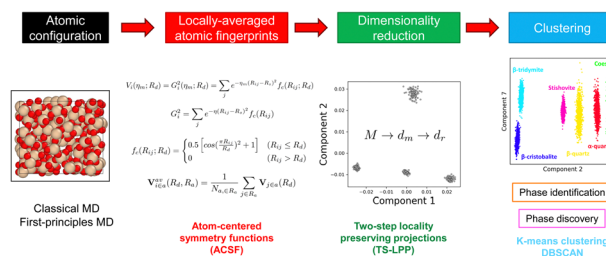
Ying Zhu, Zhiyu Huang, Jiangbin Su and Bin Tang*



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Extraction of local structure differences in silica based on unsupervised learning

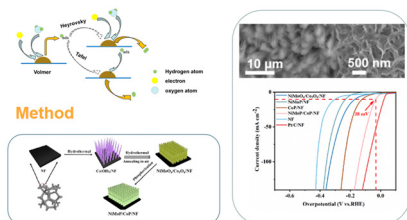
Anh Khoa Augustin Lu,* Jianbo Lin, Yasunori Futamura, Tetsuya Sakurai, Ryo Tamura* and Tsuyoshi Miyazaki*



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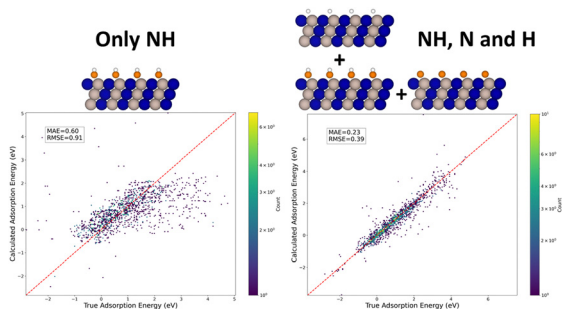
Porous tremella-like NiMoP/CoP networks electrodes as a highly effective electrocatalyst



Porous tremella-like NiMoP/CoP network electrodes as an efficient electrocatalyst

Jianzhi Wang, Jie Yang, Fuhua Huang, Yuru Li, Yu Luo, Yanan Xue, Ning Cai, Hui Li* and Faquan Yu*

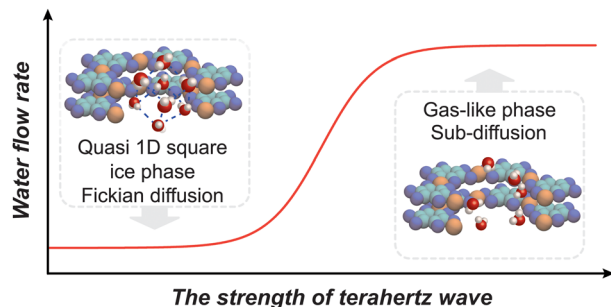
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Accessing the usefulness of atomic adsorption configurations in predicting the adsorption properties of molecules with machine learning

Walter Malone,* Johnathan von der Heyde and Abdelkader Kara

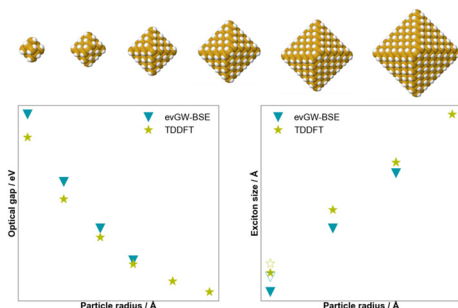
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Enhanced water permeation through the terahertz-induced phase and diffusion transition in metal–organic framework membranes

Zhi Zhu, Lei Wang, Shaojian Yan, Qilin Zhang* and Hui Yang*

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The effect of particle size on the optical and electronic properties of hydrogenated silicon nanoparticles

Eimear Madden and Martijn A. Zwijnenburg*

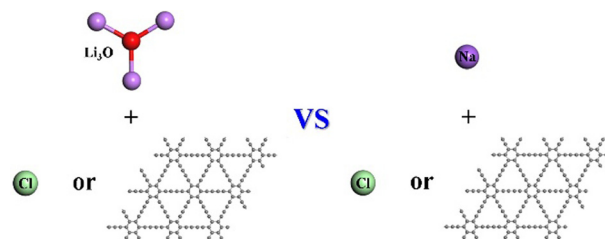


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Chemical properties of superatomic Li_3O clusters from a density functional theory perspective: formation of chloride and adsorption behavior on graphynes

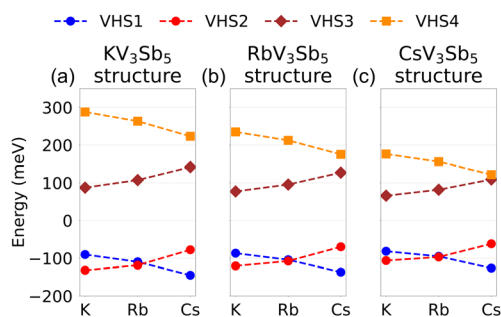
Xiao Wang, Meng Zhang* and Wei Cao*



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Chemical effect on the Van Hove singularity in superconducting kagome metal AV_3Sb_5 ($\text{A} = \text{K}, \text{Rb}, \text{and Cs}$)

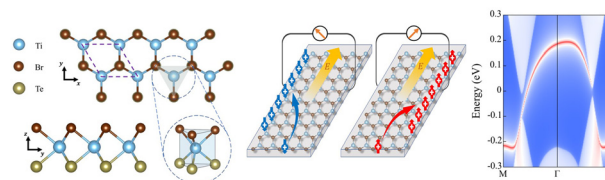
Sangjun Sim, Min Yong Jeong, Hyunggeun Lee, Dong Hyun David Lee and Myung Joon Han*



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Large valley polarization and the valley-dependent Hall effect in a Janus TiTeBr monolayer

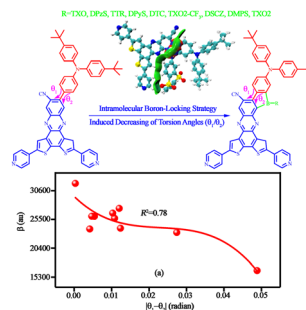
Bingwen Su,* Xiao Peng, Zhibo Yan, Lin Lin, Xiaokun Huang and Jun-Ming Liu



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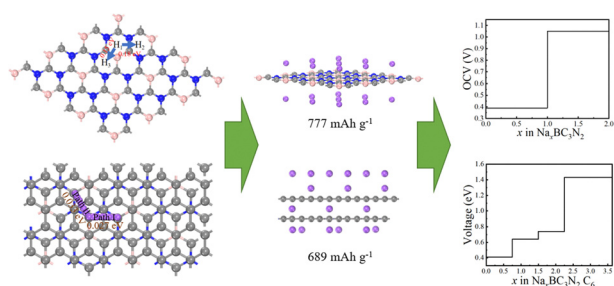
Intramolecular boron-locking strategy induced remarkable first hyperpolarizability: role of torsion angles between donor and acceptor units

Bo Li, Shichen Lin and Feng Long Gu*



RESEARCH PAPERS

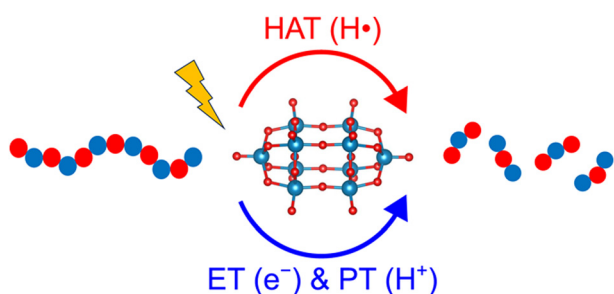
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A first-principles study of the BC_3N_2 monolayer and a BC_3N_2 /graphene heterostructure as promising anode materials for sodium-ion batteries

Xiao-Juan Ye, Rui Zhao, Xin Xiong, Xiao-Han Wang and Chun-Sheng Liu*

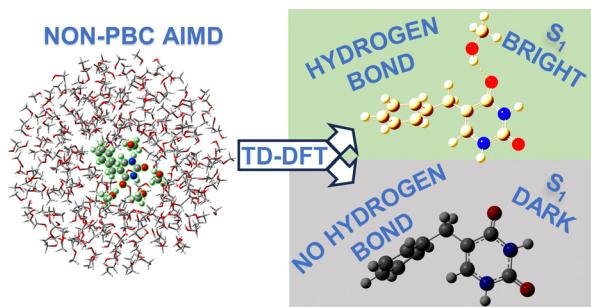
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A density functional study of the photocatalytic degradation of polycaprolactone by the decatungstate anion in acetonitrile solution

Noriyuki Minezawa, Kosuke Suzuki and Susumu Okazaki*

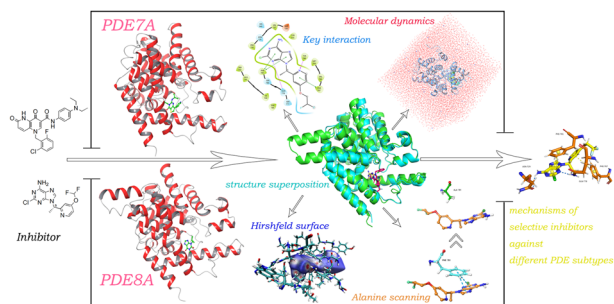
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Photophysics of a nucleic acid–protein crosslinking model strongly depends on solvation dynamics: an experimental and theoretical study

Gabriele Iuzzolino, Fulvio Perrella, Mohammadhassan Valadan, Alessio Petrone, Carlo Altucci and Nadia Rega*

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Uncovering the selectivity mechanism of phosphodiesterase 7A/8A inhibitors through computational studies

Zhijian Wang, Shizun Wang, Hanxun Wang, Baichun Hu, Zhuo Qi, Yaming Zhang, Pengfei Song, Qingkui Cai, Huali Yang* and Jian Wang*

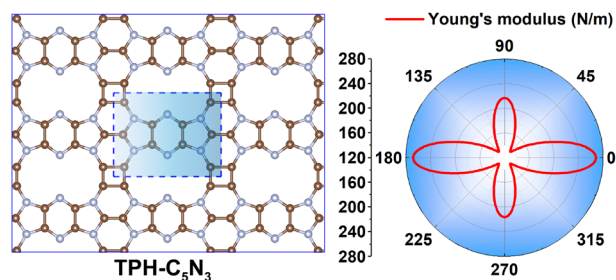


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11782

Strong mechanical anisotropy and an anisotropic Dirac state in 2D C_5N_3

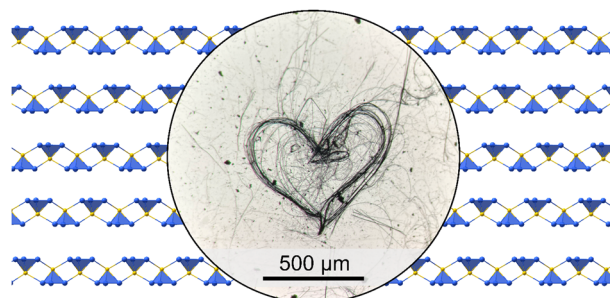
Rui Tan, Xueqing Chen, Liyufen Dai, Yulou Ouyang, Liemao Cao, Zhenkun Tang, Ming Ma, Xiaolin Wei* and Gaokuo Zhong*



11789

Electronic structure and transport in the potential Luttinger liquids $CsNb_3Br_7S$ and $RbNb_3Br_7S$

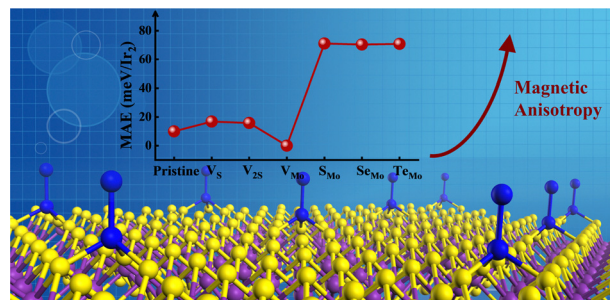
Fabian Grahlow, Fabian Strauß, Marcus Scheele, Markus Ströbele, Alberto Carta, Sophie F. Weber, Scott Kroeker, Carl P. Romao* and H.-Jürgen Meyer*



11798

Enhanced magnetic anisotropy of iridium dimers on antisite defects of two-dimensional transition-metal dichalcogenides

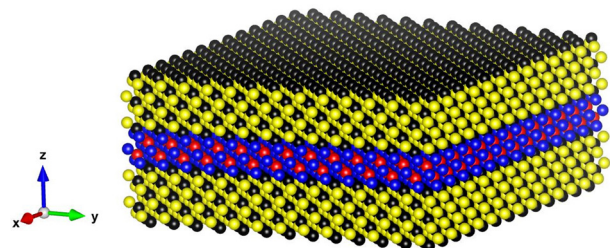
Jun Wang, Chen Yao, Siqi Lu, Suyun Wang, Dong Zheng, Fengqi Song and Jianguo Wan*



11807

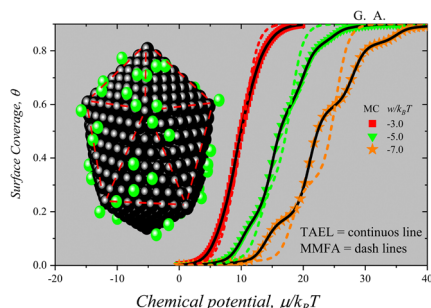
Observation of spin-splitting energies on sp–d exchange interactions tailored in colloidal CdSe/CdMnS core/shell nanoplatelets: an atomistic tight-binding model

Worasak Sukkabot



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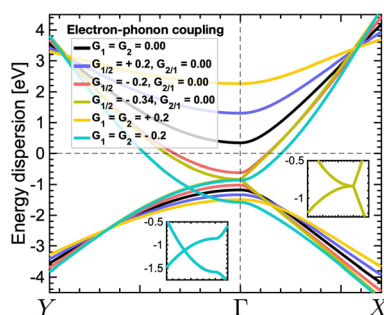
11815



Adsorption on nanoparticles with surface defects: mean field and energy level approaches

P. M. Pasinetti, J. E. Pena-Ausar and O. A. Pinto*

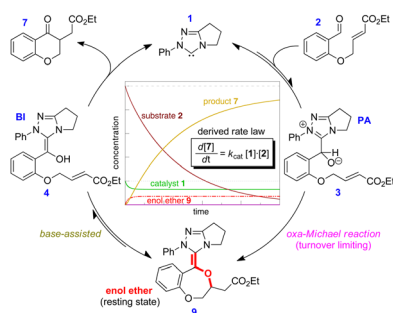
11825



Adjustment of optical absorption in phosphorene through electron-phonon coupling and an electric field

Do C. Hap, Le P. Q. Hung, Luong T. Tung, Le T. T. Phuong and Tran Cong Phong*

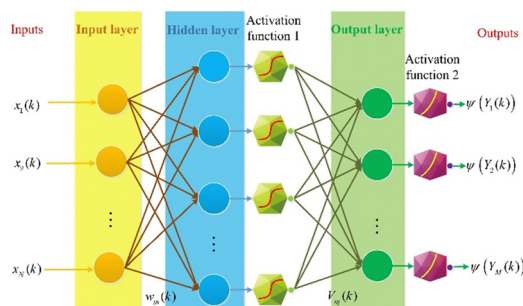
11833



Catalytic role of the enol ether intermediate in the intramolecular Stetter reaction: a computational perspective

Gou-Tao Huang and Jen-Shiang K. Yu*

11854



A novel activation function based on DNA enzyme-free hybridization reaction and its implementation on nonlinear molecular learning systems

Chengye Zou

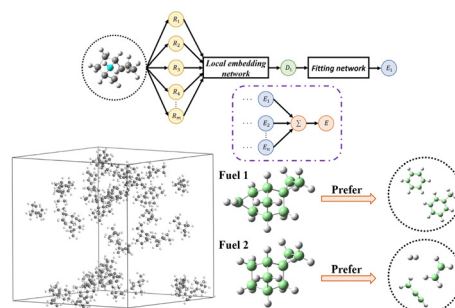


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11867

A neural network potential energy surface assisted molecular dynamics study on the pyrolysis behavior of two spiro-hydrocarbons

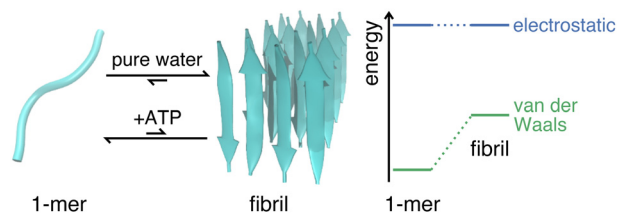
Hang Xiao and Bin Yang*



11880

How ATP suppresses the fibrillation of amyloid peptides: analysis of the free-energy contributions

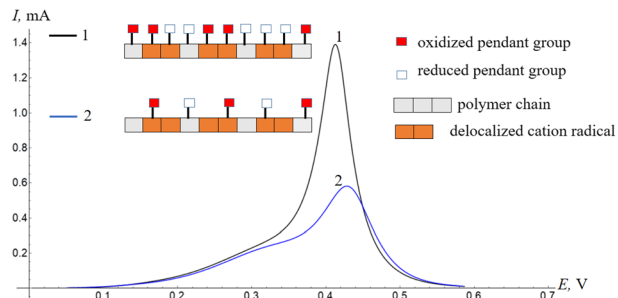
Tuan Minh Do,* Dominik Horinek and Nobuyuki Matubayasi*



11893

Thermodynamic model for voltammetric responses in conducting redox polymers

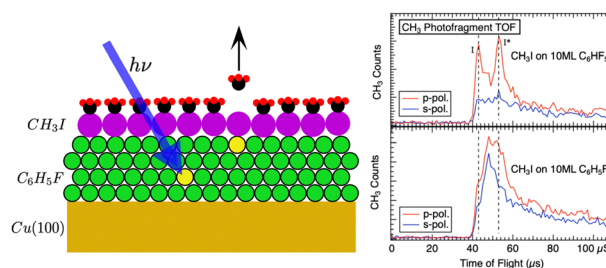
Dmitrii V. Anishchenko,* Anatolii A. Vereshchagin, Arseniy Y. Kalnin, Julia V. Novoselova, Lyubov G. Rubicheva, Vasily V. Potapenko, Daniil A. Lukyanov and Oleg V. Levin*



11910

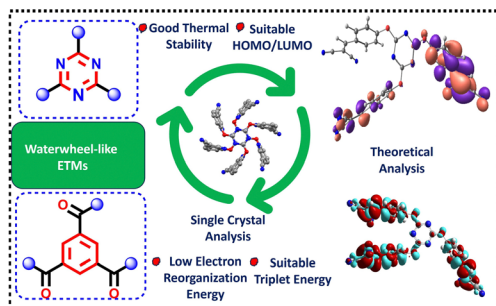
Adsorbate dissociation due to heteromolecular electronic energy transfer from fluorobenzene thin films

E. T. Jensen



RESEARCH PAPERS

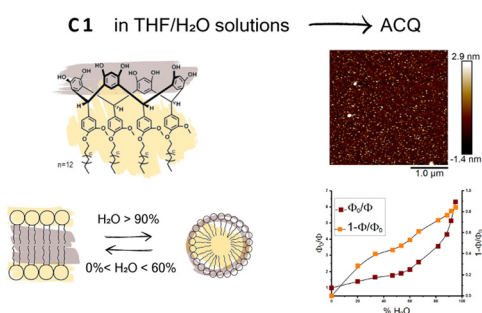
11922



Self-assembled molecular network with waterwheel-like architecture: experimental and theoretical evaluation toward electron transport capabilities for optoelectronic devices

Krishan Kumar,* Anirban Karmakar, Diksha Thakur, Dipanshu Sharma, Feng-Rong Chen, Varsha Verma, Mangey Ram Nagar, Jwo-Huei Jou,* Subrata Banik* and Subrata Ghosh*

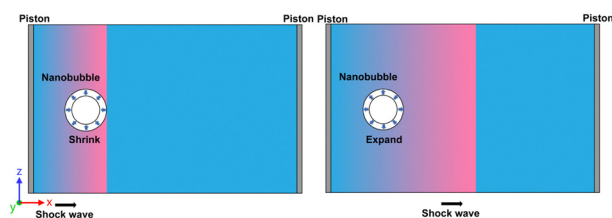
11933



The effect of water in THF/water mixtures on CMC, aggregation sizes, and fluorescence quenching of a new calix[4]resorcinarene macrocycle

María Virginia Sosa, Kashif Hussain, Eduardo D. Prieto, Tatiana Da Ros, M. Raza Shah and Ezequiel Wolcan*

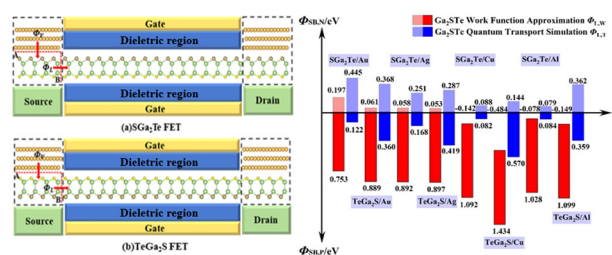
11945



The impact of low-velocity shock waves on the dynamic behaviour characteristics of nanobubbles

Ding Ma, Xiaohui Zhang,* Rensong Dong and Hua Wang

11958



First-principles studies on the electronic and contact properties of monolayer Ga₂STe-metal contacts

Wanyunfei Zhang, Cai-Juan Xia,* Xu-Mei Zhao, Guo-Qing Zhang, Lian-Bi Li, Yao-Heng Su and Qing-Long Fang



Microstructure regulation and microwave absorption properties of ZnO/RGO composites

The diagram illustrates the synthesis of ZnO nanocomposites on GO. The process begins with the dispersion of GO in deionized water. Zn²⁺ ions and a ZnO precursor are then added and stirred. Finally, thermal treatment is applied, leading to the nucleation and growth of ZnO nanoparticles on the GO surface. The legend identifies the components: Deionized water (grey), Absolute ethyl alcohol (blue), C (black), Zn²⁺ (red), Precursor of Zinc oxide (green), GO (orange), OH⁻ (yellow), Zinc oxide nanoparticle (blue star), and RGO (grey).

Understanding 2p core-level excitons of late transition metals by analysis of mixed-valence copper in a metal–organic framework

The diagram illustrates the energy levels of Cu₂O. At the top, the Cu-CO antibonding orbital is shown with molecular orbital diagrams. Below this, the conduction band minimum (CBM) and valence band maximum (VBM) are indicated. An in-gap state is located between the CBM and VBM. The exciton binding energy is the energy difference between the CBM and the in-gap state. The first main peak is at the VBM. The pre-edge peak is at the Cu²⁺ 2p level. The Cu⁺ 2p level is shown below the Cu²⁺ 2p level. The 2p orbital energy difference is the energy difference between the Cu⁺ 2p and Cu²⁺ 2p levels. An X-ray source is shown emitting a beam towards the Cu²⁺ 2p level.

Counterion effects on the mesomorphic and electrochemical properties of guanidinium salts

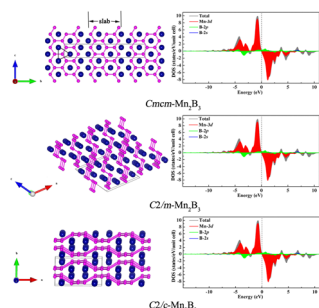
Isomerization of surface functionalized SWCNTs and the critical influence on photoluminescence: static calculations and excited-state dynamics simulations

Stable configuration?
Photoluminescent?

The diagram illustrates the photoluminescence mechanism in a carbon nanotube. The top row shows the 'Stable configuration?' (left) and 'Photoluminescent?' (right) states. The bottom row shows the 'Stable configuration?' (left) and 'Photoluminescent?' (right) states. The photoluminescent states show the formation of a radical cation (P⁺) and a radical anion (P⁻) on the nanotube surface, which are stabilized by chlorine atoms.

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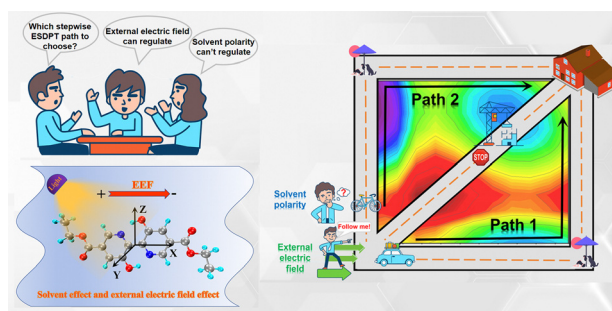
12009



First-principles study of multifunctional Mn_2B_3 materials with high hardness and ferromagnetism

Chunhong Xu,* Kuo Bao, Sheng Wang, Gang Wu, Shuailong Ma, Liangliang Li, Paul K. Chu and Chao Liu*

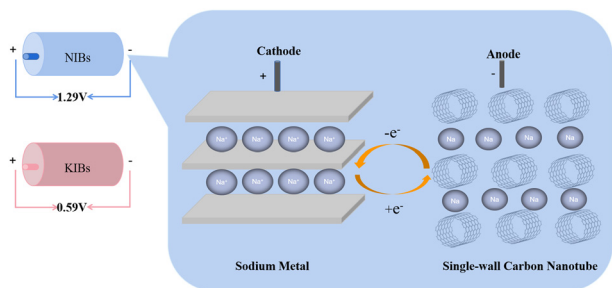
12016



Regulating and controlling the stepwise ESDPT channel of $\text{BP(OH)}_2\text{DCEt}_2$ using the strategy of solvent polarity and external electric field

Hongbin Zhuang, Wei Shi, Guijie Zhao and Yongqing Li*

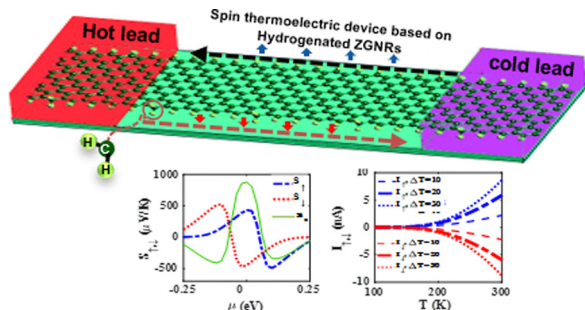
12027



Optimizing cell voltage dependence on size of carbon nanotube-based electrodes in Na-ion and K-ion batteries

Xia Liu, Jiacheng Gong, Yizhi Jiang, Xiao He* and Jinrong Yang*

12035



Spin thermoelectric properties induced by hydrogen impurities in zigzag graphene nanoribbons

Somaye Esteki and Rouhollah Farghadan*

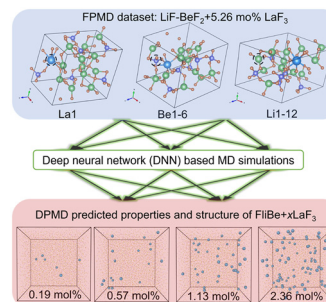


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12044

Compositional transferability of deep potential in molten LiF–BeF₂ and LaF₃ mixtures: prediction of density, viscosity, and local structure

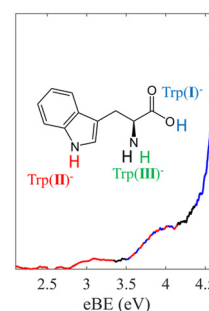
Xuejiao Li,* Tingrui Xu and Yu Gong*



12053

Photoelectron spectroscopy of the deprotonated tryptophan anion: the contribution of deprotomers to its photodetachment channels

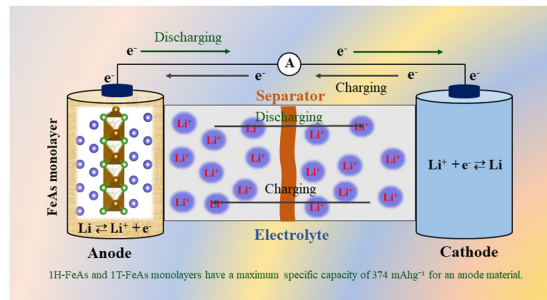
Jemma A. Gibbard,* Catherine S. Kellow and Jan. R. R. Verlet



12060

Iron-arsenide monolayers as an anode material for lithium-ion batteries: a first-principles study

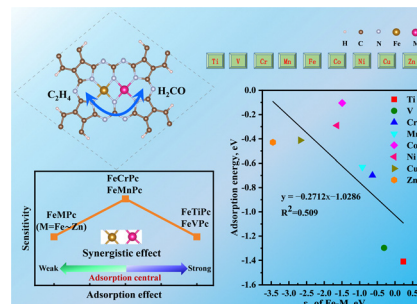
Ajay Kumar and Prakash Parida*



12070

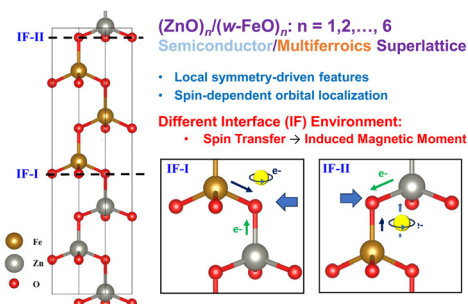
Proposals for gas-detection improvement of the FeMPc monolayer towards ethylene and formaldehyde by using bimetallic synergy

Yingying Ma, Huihui Xiong* and Jianbo Zhang



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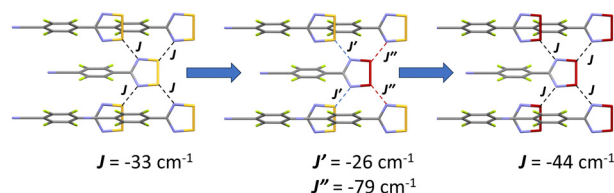
12084



Local symmetry-driven interfacial magnetization and electronic states in (ZnO)_n/(w-FeO)_n superlattices

Jia-Xin Gao, Yi Sheng Ng, Hao Cheng, Hui-Qiong Wang,* Tie-Yu Lü* and Jin-Cheng Zheng*

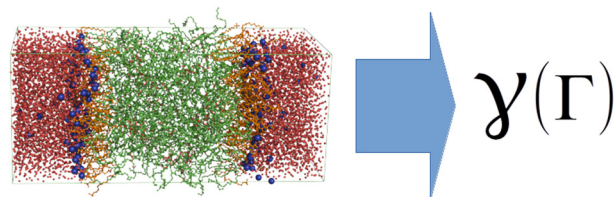
12097



Towards molecular alloys: computational and experimental studies on (p-NCC₆F₄CNSeSeN)_x(p-NCC₆F₄CNSSN)_{1-x}

Asli M. Wehelie, Lara K. Watanabe, Bin Zhang, Sahar Nikoo and Jeremy M. Rawson*

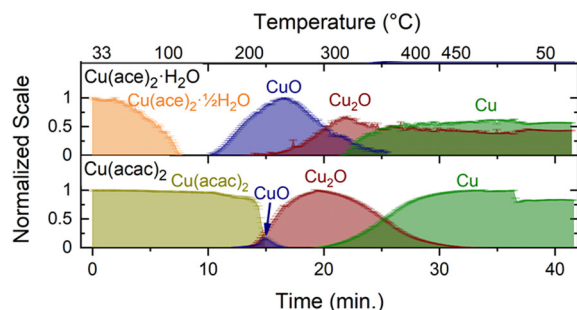
12107



Computational predictions of interfacial tension, surface tension, and surfactant adsorption isotherms

Jing Li, Carlos Amador and Mark R. Wilson*

12121



Exploration of anion effects in solvothermal synthesis using *in situ* X-ray diffraction

Nils Lau Nyborg Broge, Andreas Dueholm Bertelsen, Ida Gjerlevsen Nielsen, Magnus Kløve, Martin Roelsgaard, Ann-Christin Dippel, Mads Ry Vogel Jørgensen and Bo Brummerstedt Iversen*

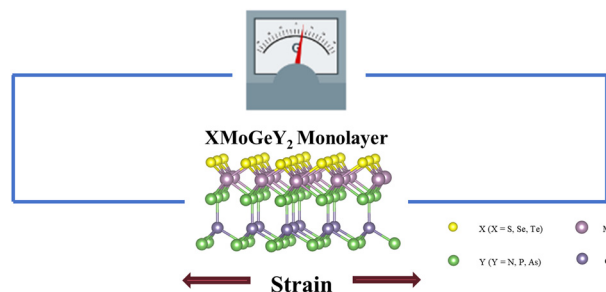


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12133

Asymmetric XMoGeY_2 ($\text{X} = \text{S, Se, Te}$; $\text{Y} = \text{N, P, As}$) monolayers as potential flexible materials for nano piezoelectric devices and nanomedical sensors

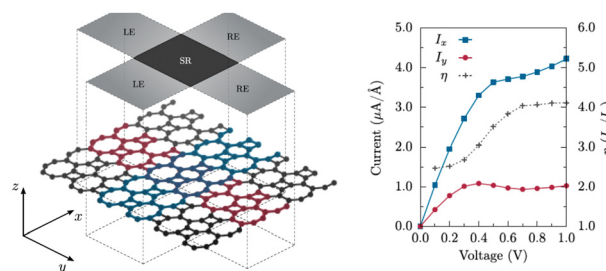
Zujun Li, Jiasheng Luo, Yushan Zhou, Jiawei Chen, Haojun Ling, Jun Zeng, Yujue Yang and Huafeng Dong*



12142

Directional dependence of the electronic and transport properties of biphenylene under strain conditions

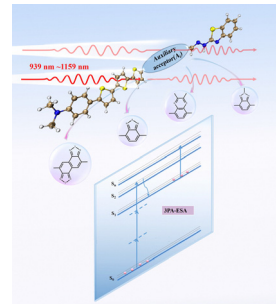
Danilo P. Kuritza, Roberto H. Miwa and José Eduardo Padilha*



12150

Intramolecular charge transfer enhanced optical limiting in novel hydrazone derivatives with a $\text{D}_1\text{-D-A}_1\text{-}\pi\text{-A}$ structure

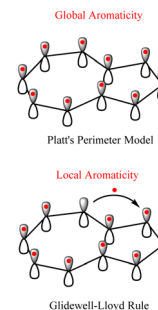
Hongjuan Zhu, Danyang Zhang, Xianghao Sun, Shifeng Qian, Eryin Feng and Xiaowei Sheng*



12162

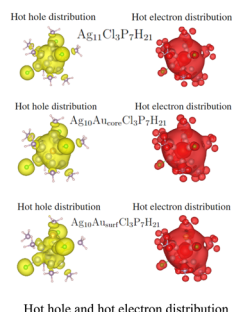
Is azulene's local aromaticity and relative stability driven by the Glidewell–Lloyd rule?

Rodrigo Báez-Grez and Ricardo Pino Rios*



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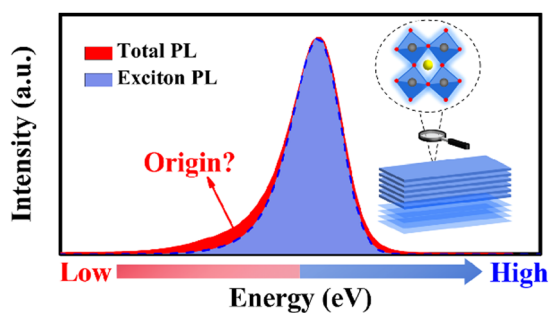
12168



The impact of a dopant atom on the distribution of hot electrons and holes in Au-doped Ag nano-clusters

Junais Habeeb Mekkath

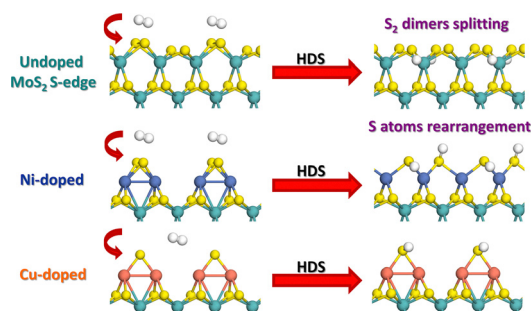
12179



Origin of the low-energy tail in the photoluminescence spectrum of CsPbBr₃ nanoplatelets: a femtosecond transient absorption spectroscopic study

Jinwei Liu, Rong Lu and Anchi Yu*

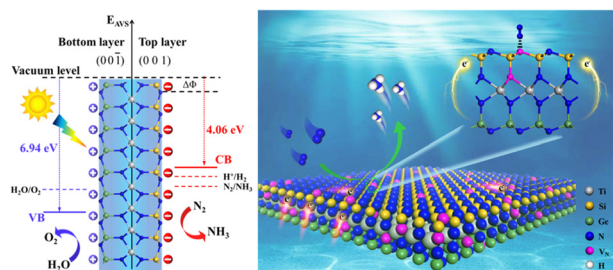
12188



Theoretical insight into the rearrangement of sulfur atoms on the Ni- and Cu-doped MoS₂ S-edge induced by hydrogen adsorption under HDS reaction conditions

Alba B. Vidal,* Oscar Hurtado-Aular, José Luis Peña-Mena, Rafael Añez and Anibal Sierraalta

12199



A novel two-dimensional Janus TiSiGeN₄ monolayer with N vacancies for efficient photocatalytic nitrogen reduction

Zhe Sun, Rongfeng Guan, Huimin Li, Shilong Feng, Lin Ma, Qianqian Shen,* Lixia Ling, Husheng Jia and Jinbo Xue*

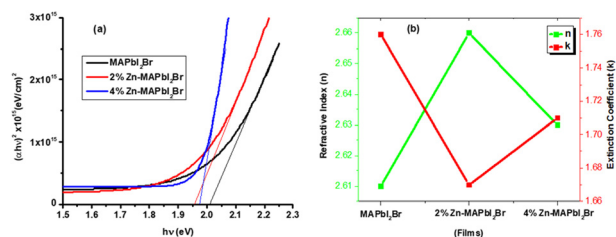


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12210

The structural, optical and photovoltaic properties of Zn-doped MAPbI₂Br perovskite solar cells

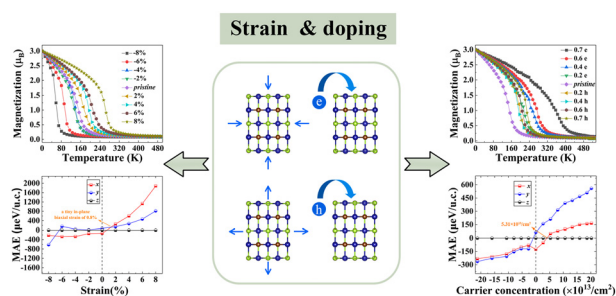
M. I. Khan,* Saddam Hussain,* Badriah S. Almutairi,
A. Dahshan, Ali Mujtaba and Syed Muhammad Ahmad



12219

Enhanced ferromagnetism, perpendicular magnetic anisotropy and high Curie temperature in the van der Waals semiconductor CrSeBr through strain and doping

Ruilin Han,* Xiaomin Xue and Peng Li



12231

Laser power and high-temperature dependent Raman studies of layered bismuth and copper-based oxytellurides for optoelectronic applications

Prabhukrupa C. Kumar, Subrata Senapati,*
Monalisa Pradhan, Gopal K. Pradhan and
Ramakanta Naik*

