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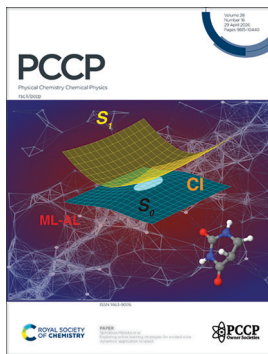
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Cover

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Inside cover

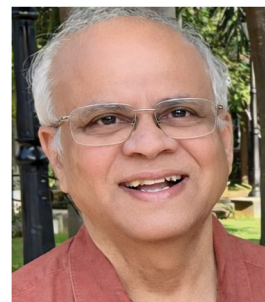
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PROFILE

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Atomic and molecular collisions: classical and quantum dynamics, chaos and fractals, periodic orbits, quantum mechanical resonances, gas-surface scattering, atomic and molecular clusters, atoms and molecules under confinement: a kaleidoscopic view

Narayanasami Sathyamurthy

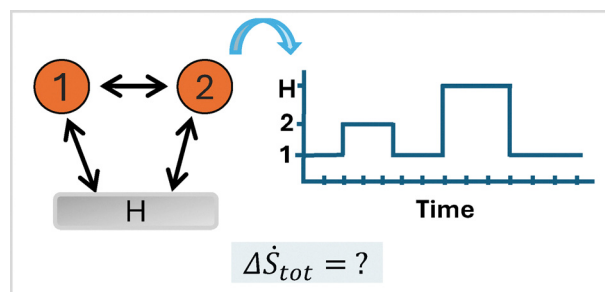


REVIEWS

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Identification and quantification of irreversibility in stochastic systems

Aishani Ghosal and Gili Bisker*



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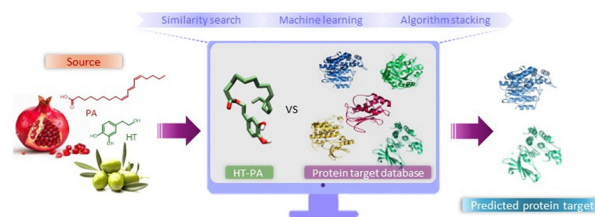


REVIEWS

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Integrative reverse-screening approaches for target discovery: the case of hydroxytyrosyl punicate

James Stewart, Meriem Chayah and Carmen Domene*

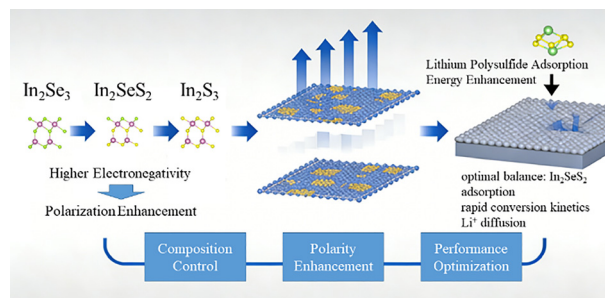


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Tailoring ferroelectric polarization in $\text{In}_2\text{Se}_n\text{S}_{3-n}$ monolayers via Se/S ratio modulation to boost polysulfide electrocatalysis

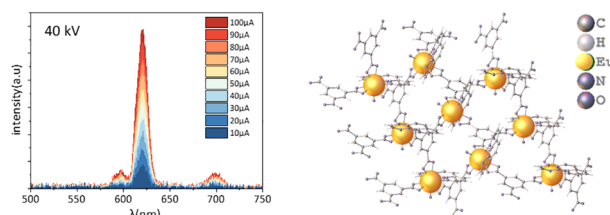
Haoyun Dou, Xuanpan Xu, Rawaid Ali, Hongqing Ma,* Chen Qing* and Hong-En Wang*



9891

Cathodo- and X-ray excited luminescence of europium tri- and tetracarboxybenzoates and phenanthroline

Yiming Yin, Dmitrii Kopytov, Anastasiya Parashuk, Alexander S. Goloveshkin, Egor Latipov, Guo Zhipeng, Ivan Khanbekov, Yanan Zhu and Valentina V. Utochnikova*

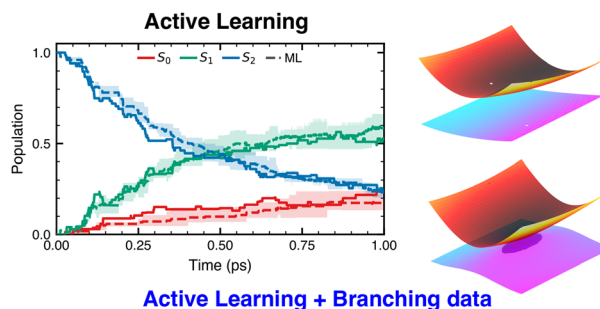


RESEARCH PAPERS

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Exploring active learning strategies for excited state dynamics: application to uracil

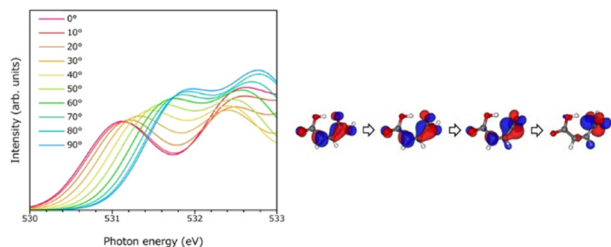
Juan Carlos San Vicente Veliz, Mark DelloStritto and Spiridoula Matsika*



Active Learning + Branching data



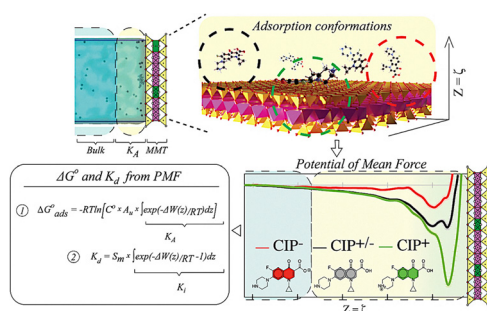
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Controlling the pH of aqueous succinic and maleic acids analyzed by X-ray absorption spectroscopy

Risa Okada, Rikuya Adachi, Ryosuke Yamamura, Taiga Suenaga, Takashi Tokushima, Yuka Horikawa, Masaki Oura and Osamu Takahashi*

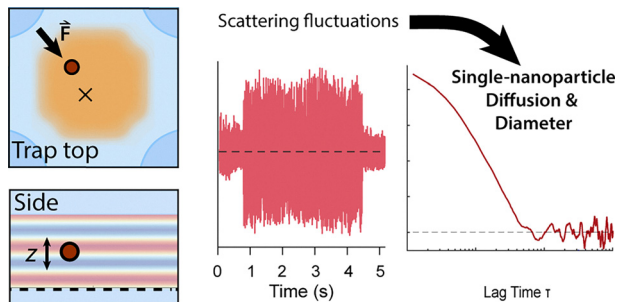
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Molecular dynamics simulations of pH-dependent ciprofloxacin adsorption to Na-montmorillonite

Rogers E. Swai and Michael Holmboe*

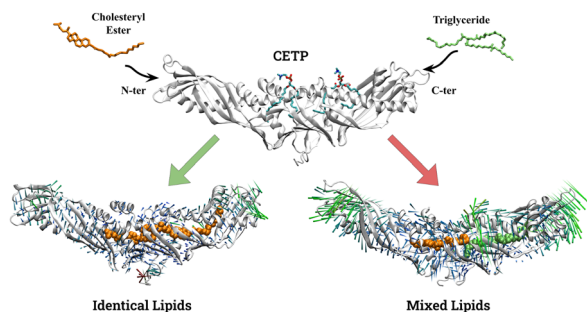
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Sizing single trapped nanoparticles with interferometric scattering fluctuations

Abhijit A. Lavania and William B. Carpenter*

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Beyond the crystal: molecular dynamics investigations of CETP with varied lipid substrates reveal asymmetric dominant motions

Bharath Raj Parthasarathy and Sanjib Senapati*

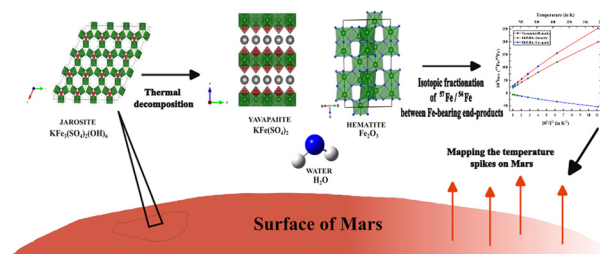


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Decoding episodes of past temperature spikes on the Martian surface using jarosite

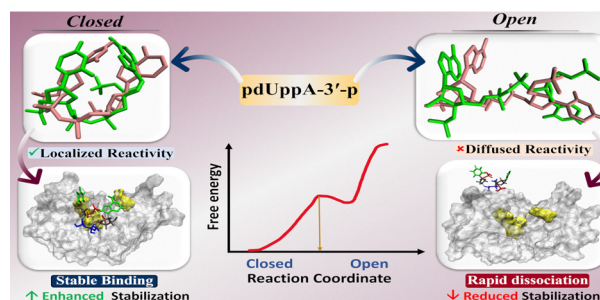
Debdatta Banerjee and Swastika Chatterjee*



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Exploring the conformation-dependent reactivity and dynamics of a dinucleotide inhibitor of ribonuclease A

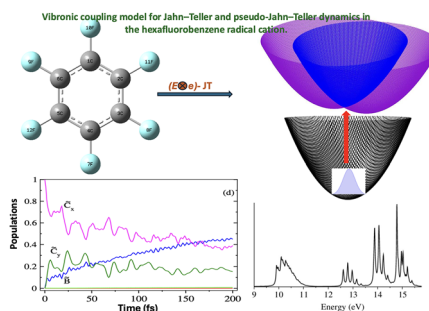
Sudipti Priyadarsinee, Arunendu Das* and Srabani Taraphder*



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The Jahn–Teller and pseudo-Jahn–Teller effects in hexafluorobenzene radical cation: nonradiative decay and radiative emission

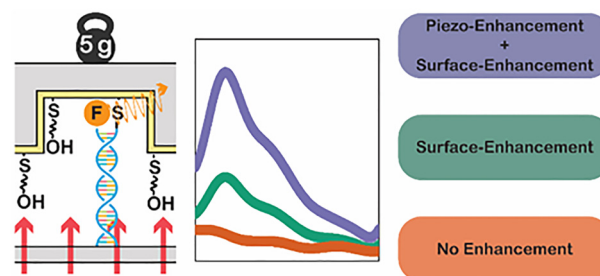
Arun Kumar Kanakati,* Vadala Jhansi Rani and S. Mahapatra*



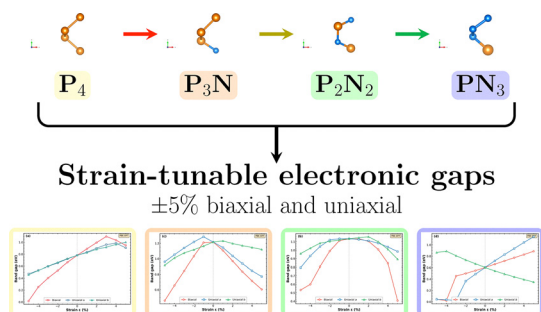
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Dual-enhanced fluorescent biosensors using metal-coated piezoelectric nanoimprinted substrates

Ghadeer Almohammadi, Dominik Duleba, Aeshah F. Alotaibi, Eni Kume, Adrià Martínez-Aviñó, James H. Rice* and Robert P. Johnson*



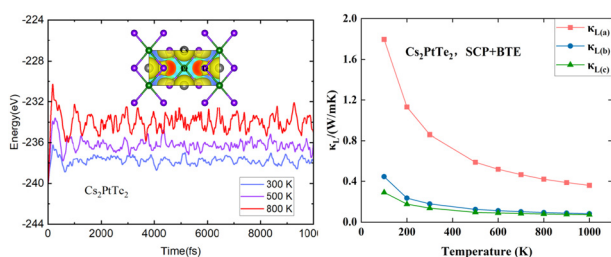
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Electronic tunability and anisotropy in 2D P–N allotropes under strain

Mohammed Benchtaï,* Abdellah Sellam, Abderrahim Bakak, Driss Lahboub, Abdelaziz Koumina, Mohamed Lotfi and Rodolphe Heyd

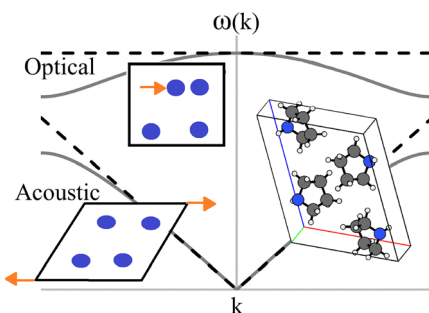
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High thermoelectric performance induced by quasi-one-dimensional structure in X(Cs & Rb)₂PtTe₂

Ziyi Pan, Weiyu Zhou, Qinheng Li, Xiang Yan, Jinpeng Yang* and Shuming Zeng*

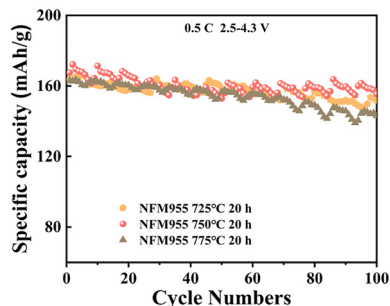
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Einstein–Debye model for density-functional prediction of vibrational free energies of molecular crystals

Cameron J. Nickerson and Erin R. Johnson*

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Ultrahigh-Ni cobalt-free ternary cathode LiNi_{0.9}Fe_{0.05}Mn_{0.05}O₂: synthesis and electrochemical performance for high-energy density lithium-ion batteries

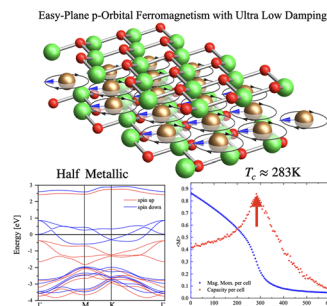
Jiatai Wang,* Siyu Dong,* Jiting Li, Cheng Qing, Guibang Zhang and Jian Li



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Near-room-temperature easy-plane p-orbital ferromagnetism in half-metallic monolayer La_2CO_2

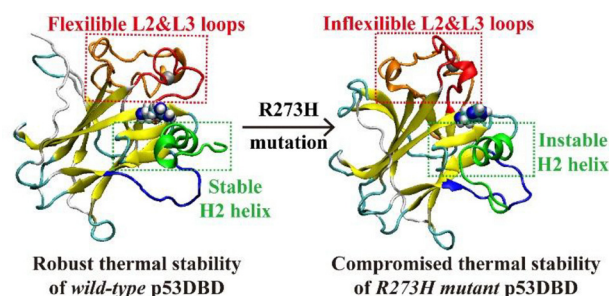
Yang Ou, Feng Tian, Yi Yang, Jianbo Zhang and Yang Zhou*



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Thermodynamic resilience of wild-type p53 DNA-binding domain and its disruption by the R273H hotspot mutation: insights from REMD simulations

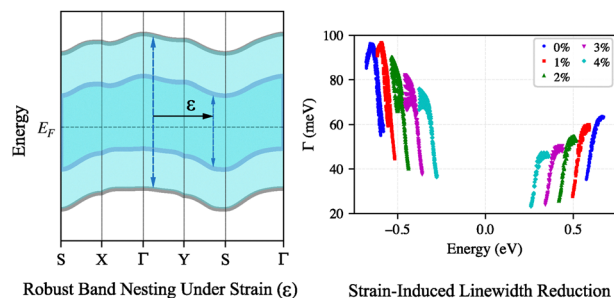
Ziqian Zhao, Gang Wang and Zhenyu Qian*



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Strain-tunable optoelectronics in a PdS_2 monolayer: the role of band nesting and carrier-phonon scattering

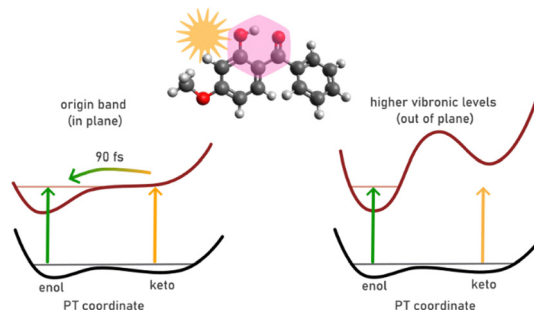
Hongfa Wang, Yancheng Gong, Subrahmanyam Pattamatta, Junwen Li, Hailong Wang* and Zhizi Guan*



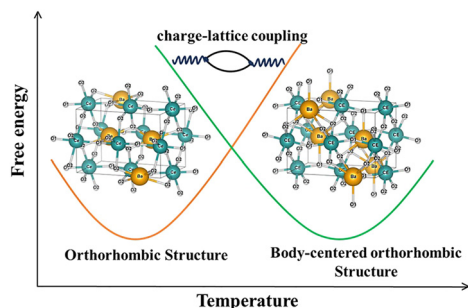
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Unexpected shortening of the excited state lifetime of oxybenzone radical cation upon excitation of the band origin

Juan C. Latorre, Franco L. Molina, Satchin Soorkia, Michel Broquier, Gilles Grégoire* and Gustavo A. Pino*



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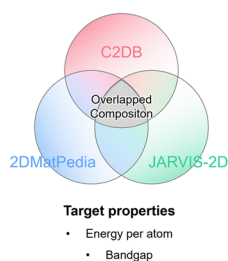


Exploring the role of charge–lattice coupling in the structural phase transition in BaCeO₃

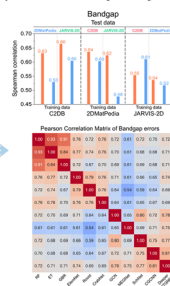
Nikita Jain, Payal Ratnawat, Archana Sagdeo* and Pankaj R. Sagdeo

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1) Practical OOD setting



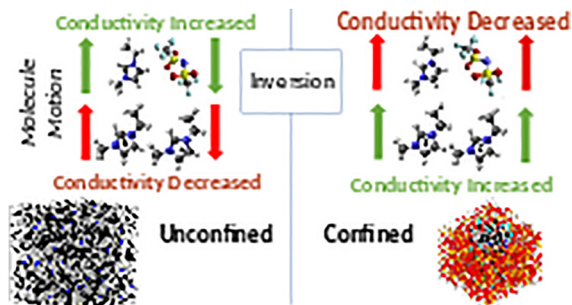
2) Transferability analysis



Comparative assessment of composition- and structure-based surrogate models across 2D materials databases

Inhyo Lee, Hyeokjae Chae, Jongwon Park, Jihye Shin, Hugon Lee* and Seunghwa Ryu*

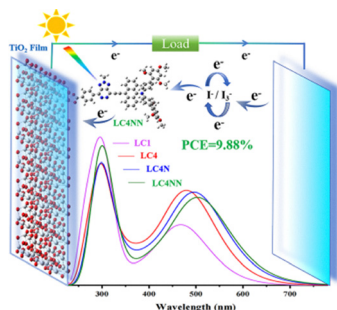
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Molecular dynamics study of [EMIM][TFSI]/(Li/Na)TFSI ionic liquids confined in silica pores

Samanvitha Kunigal Vijaya Shankar, Chris Ewels, Jean Le Bideau and Yann Claveau*

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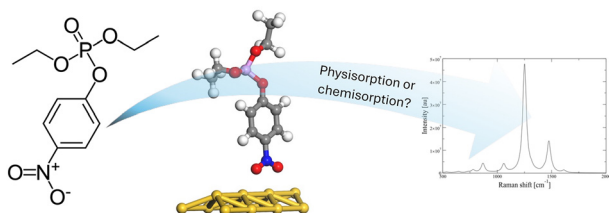


Optoelectronic performance of anthracene-based dyes with modified Hagfeldt donors in dye-sensitized solar cells

Haoyu Fan, Songfeng Li, Xiang Meng, Weiwei Pei, Tao Liu, Minxuan Wang and Yuanzuo Li*



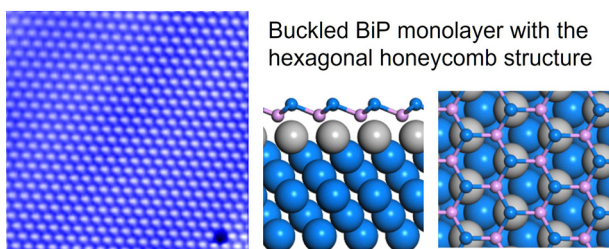
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Organophosphate ethyl paraoxon on Ag and Au surfaces: a density functional theory perspective

Hang Hu,* Jiří Hostaš,* Mohammad Sajjad Ghaemi, Junan Lin, Shiliang Wang, Anguang Hu and Hsu Kiang Ooi

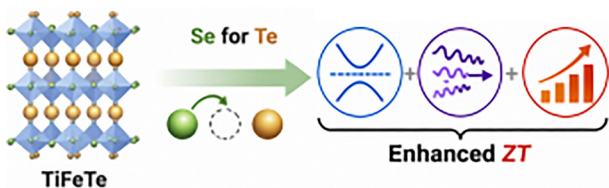
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Epitaxial growth of a buckled BiP monolayer on Bi(111)

Ting-Ting Zhang, Gang Yao,* Xiao-Tian Yang, Kai Sun, Ji-Yong Yang, Min-Long Tao, Hua-Xing Zhu and Jun-Zhong Wang*

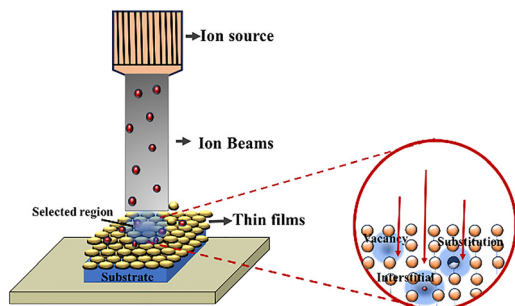
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Alloying-induced reduction of lattice thermal conductivity in TiFeTe

Lei Gao,* Ruixiu Liu, Yaoyao Chu, Zhen Luan, Yushan Li and Xing Xiong

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Enhancement of the electrochemical properties of BiVO₄: the role of oxygen vacancies induced by Ag ion implantations

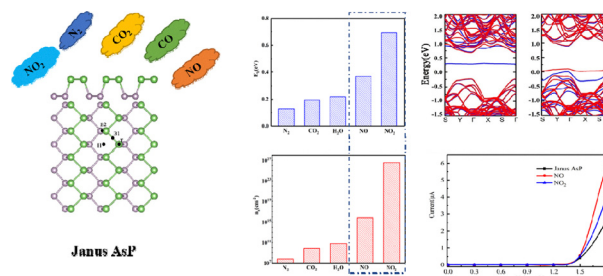
Shilpa Chauhan, Richa Saini, Thanigai Arul Kumaravelu, Chung-Li Dong, K. Deva Rani Devi and Asokan Kandasami*



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Janus AsP monolayers: a promising 2D platform for NO and NO₂ gas sensing

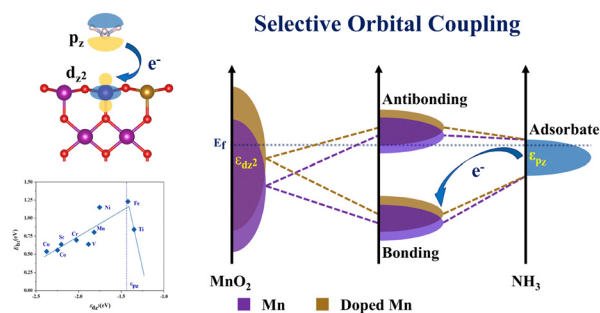
Yuncai Jiang, X. Tao, C. Hung, Shuangying Lei* and Zaifa Zhou*



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Elucidating d–d orbital hybridization in metal-doped MnO₂ for the inhibition of N₂O formation in NH₃–SCR

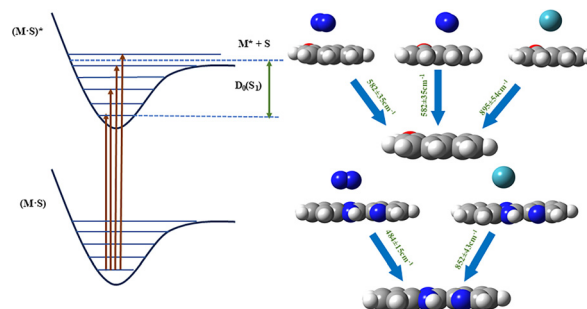
Kai Xie, Ying Wang, Fenghui Li, Haiqiao Wei and Lei Zhou*



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Determination of the intermolecular dissociation energies in the dispersion-bound N₂ and Xe complexes of 2-(2'-pyridyl)benzimidazole and 1-naphthol

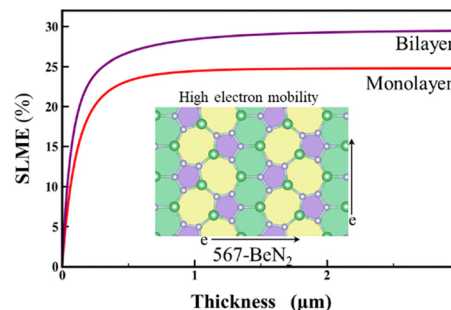
Bhavika Kalal, Simran Baweja, Satish Bhusan Panda and Surajit Maity*



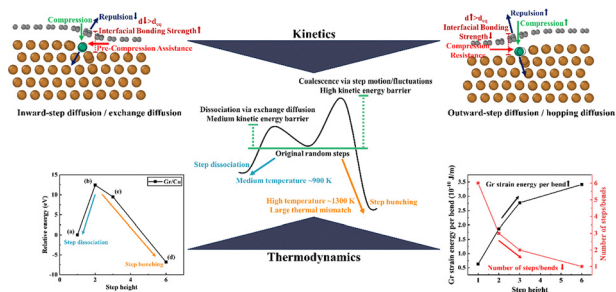
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A direct-band-gap planar BeN₂ monolayer with high mobility and bilayer-enhanced photovoltaic efficiency

Changping Sun, Renyu Duan, Hongzhe Pan, Zhaoxin Lu, Caoping Niu,* Meiling Xu* and Yinwei



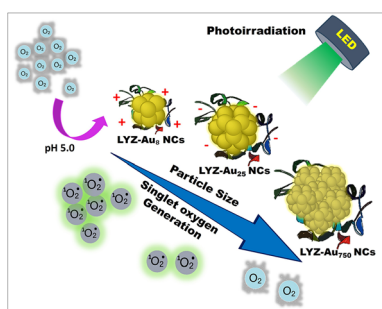
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Surface diffusion of Cu mediated by graphene coverage

Haitao Zhang, Qi Zhang, Baixue Bian,* Yue Liu,*
Tongxiang Fan* and Mingyu Gong

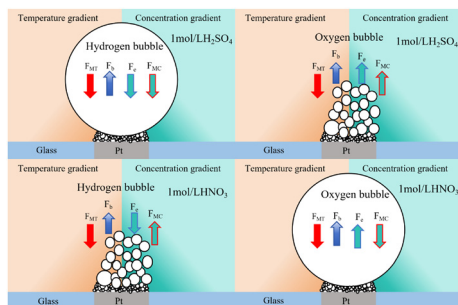
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Size-dependent properties of gold nanoclusters in photoirradiation-mediated singlet oxygen generation

S Santhoshkumar, Yan-Ru Liu and Wei-Lung Tseng*

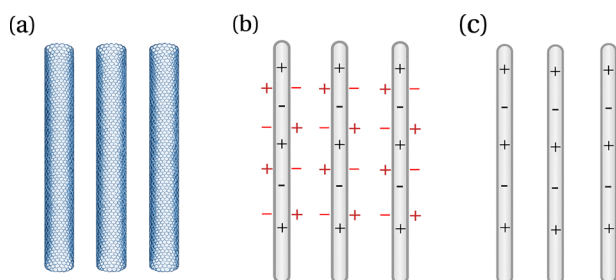
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Experimental investigation of hydrogen and oxygen bubble growth on platinum microelectrodes of different sizes

Peng Kong, Liang Hao, Ming Gao,* Wu-han Dong and
Qi-rong Zuo

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Do 1-dimensional metals prefer to form even-numbered van der Waals clusters?

S. Pal* and John F. Dobson*

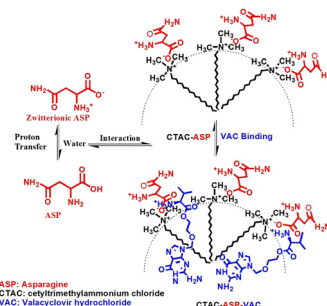


RESEARCH PAPERS

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Zwitterionic asparagine as a molecular modulator of cetyltrimethylammonium chloride micellization and drug–micelle interactions: a detailed study

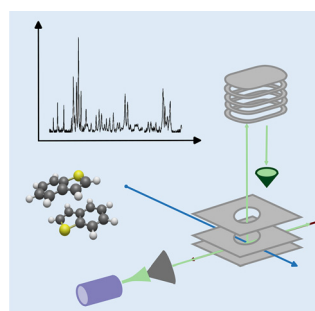
Malik Abdul Rub,* Anirudh Srivastava,* Naved Azum and Khalid A. Alzahrani



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Elucidating the structure and binding nature of thianaphthene dimers using gas-phase infrared spectroscopy

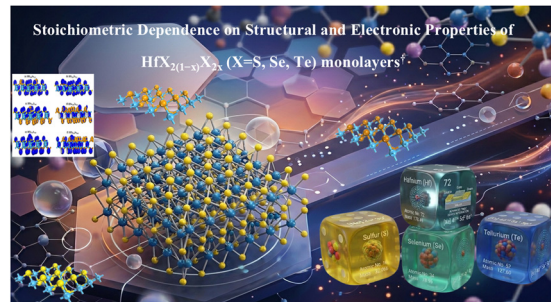
Gaia Zucali, Vincent J. Esposito, Sandra Brünken and Piero Ferrari*



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Stoichiometric dependence of the structural and electronic properties of $\text{HfX}_{2(1-x)}\text{X}_{2x}$ ($X = \text{S, Se, Te}$) monolayers

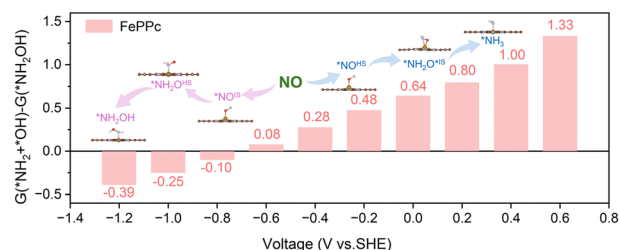
Vivek Mahajan* and Hitesh Sharma



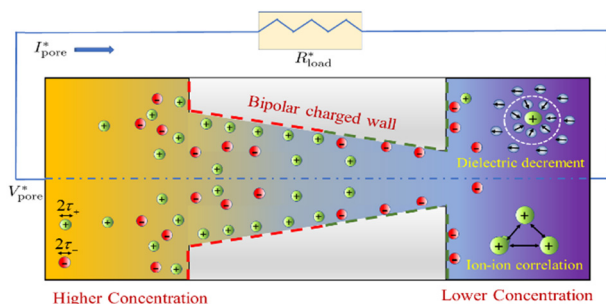
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A spin-crossover-mediated potential-dependent selective NO reduction reaction on iron-polyphthalocyanine: a DFT study

Ya Jin, Mingyuan Yu, Erjun Kan and Cheng Zhan*



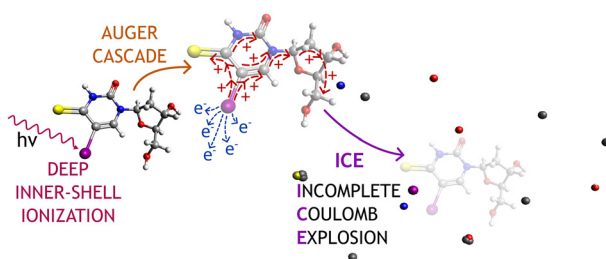
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Impact of multivalent ions on osmotic power generation in a bipolar conical pore: a numerical analysis based on modified electrokinetic models

Shakyajit Paik and Somnath Bhattacharyya*

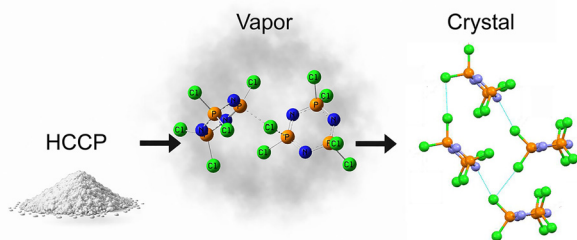
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Dissociation of halogenated deoxyridines as potential radiosensitizers, induced by deep inner-shell photoionization – experiment and modeling

Kerttu-Inkeri Pusa,* Edwin Kukk, Marta Berholts, Tatiana Marchenko, Iyas Ismail, Denis Céolin, Marc Simon and Oksana Travnikova*

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Hexachlorocyclotriphosphazene: macromolecular assemblies in vapor and crystalline phases. experimental and computational approach

Semyon S. Egorov,* Elena Yu. Tupikina and Artem A. Selyutin

