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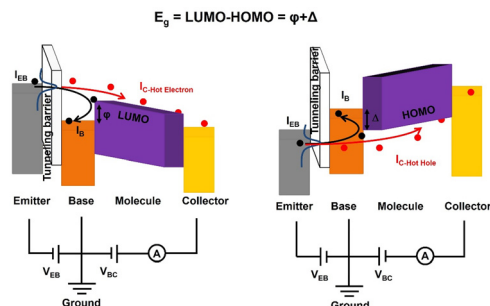


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Going ballistic: a novel characterization for the electronic energy gap

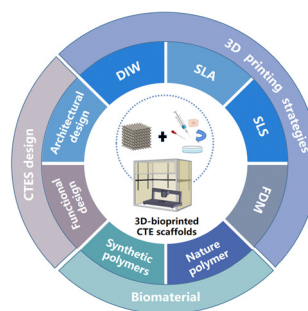
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From materials to clinical use: advances in 3D-printed scaffolds for cartilage tissue engineering

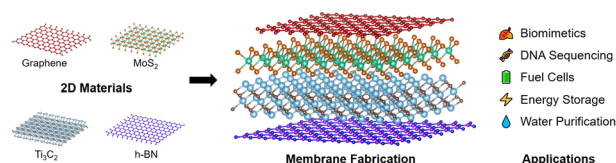
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2D materials towards energy conversion processes in nanofluidics

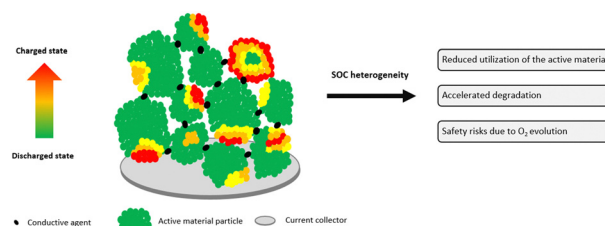
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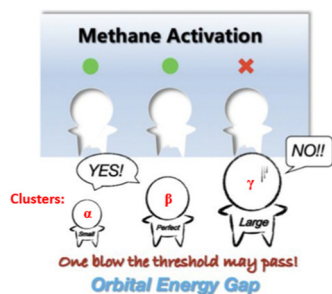
State-of-charge of individual active material particles in lithium ion batteries: a perspective of analytical techniques and their capabilities

Marc Vahnstiege, Martin Winter, Sascha Nowak* and Simon Wiemers-Meyer



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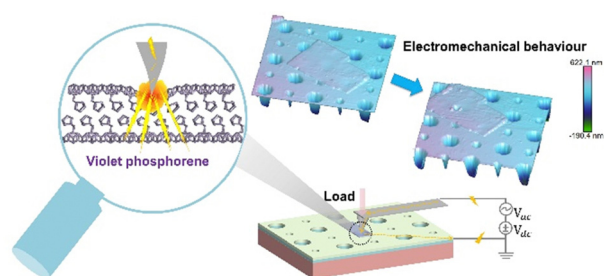
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On the performance of the M–C (M = Fe, Ru, Os) unit toward methane activation

Shihan Li, Chao Qian, Xiao-Nan Wu* and Shaodong Zhou*

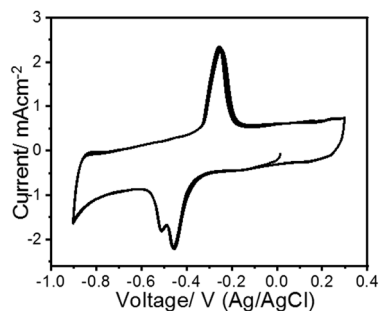
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Electromechanical behaviour of violet phosphorene nanoflakes

Bo Zhang,* Zhenyu Wang,* Chengxiang Chen, Mengyue Gu, Jun Zhou and Jinying Zhang*

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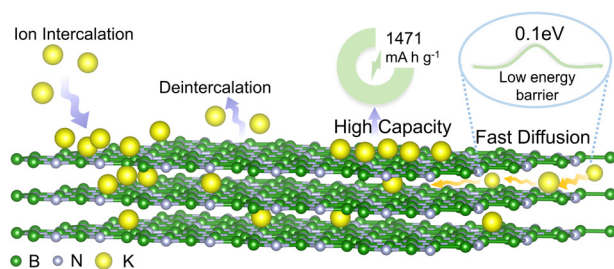


Aqueous electrolyte-mediated reversible K^+ ion insertion into graphite

Ritupurna Baishya, Devalina Sarmah, Debajyoti Mahanta and Shyamal K. Das*

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First principles study of B_7N_5 as a high capacity electrode material for K-ion batteries

Yu Xiong, Yuhang Wang, Ninggui Ma, Yaqin Zhang, Shuang Luo and Jun Fan*

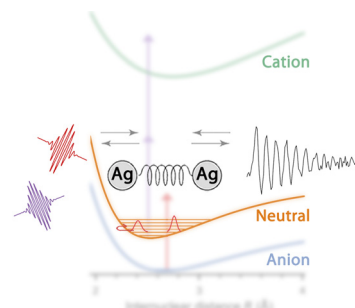


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Nuclear quantum dynamics on the ground electronic state of neutral silver dimer $^{107}\text{Ag}^{109}\text{Ag}$ probed by femtosecond NeNePo spectroscopy

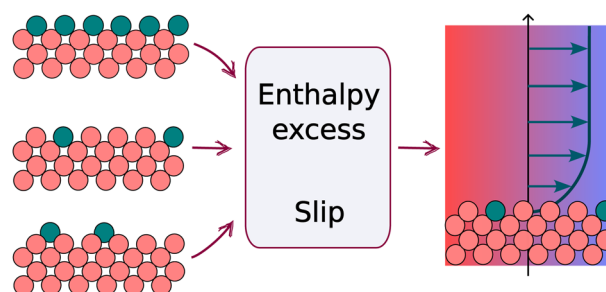
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Complex coupling between surface charge and thermo-osmotic phenomena

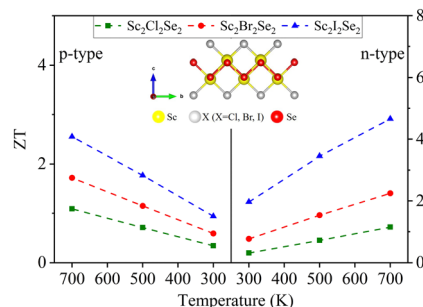
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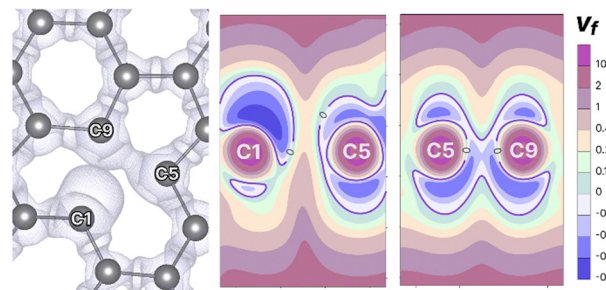
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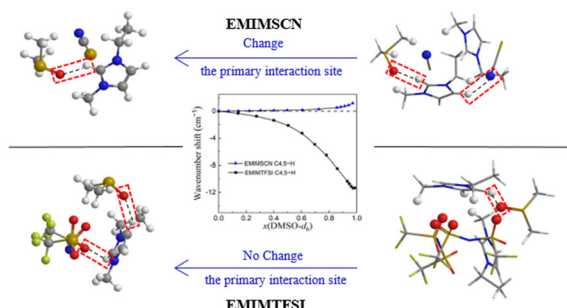
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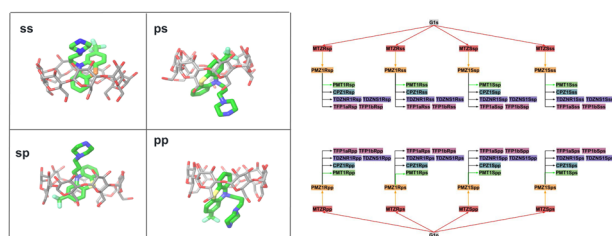
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Rui Zhao, Xianzhen Xu, Zonghua Wang, Yanzhen Zheng* and Yu Zhou*

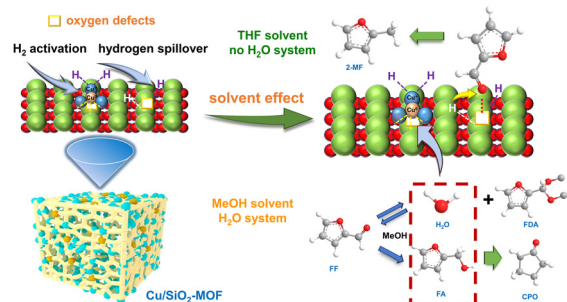
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Taming multiple binding poses in alchemical binding free energy prediction: the β -cyclodextrin host–guest SAMPL9 blinded challenge

Sheenam Khuttan, Solmaz Azimi, Joe Z. Wu, Sebastian Dick, Chuanjie Wu, Huafeng Xu and Emilio Gallicchio*

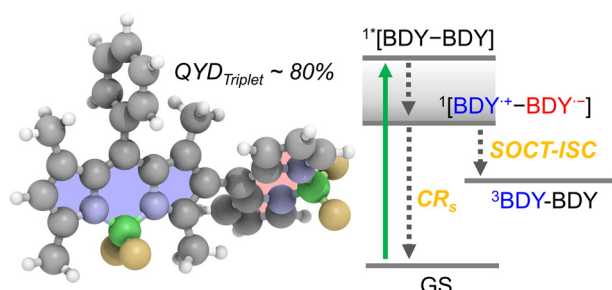
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Cu/SiO₂ synthesized with HKUST-1 as precursor: high ratio of Cu⁺/(Cu⁺ + Cu⁰) and rich oxygen defects for efficient catalytic hydrogenation of furfural to 2-methyl furan

Zhiyuan Zong, Hongzi Tan,* Pengrui Zhang, Chao Yuan, Rongrong Zhao, Feng Song, Weiming Yi, Fengshan Zhang and Hongyou Cui*

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Spin–orbit charge-transfer intersystem crossing in heavy-atom-free orthogonal covalent boron-dipyrromethene heterodimers

Zeming Wang, Lin Ma, Hongmei Zhao, Yan Wan, Xian-Fu Zhang,* Yang Li,* Zhuoran Kuang* and Andong Xia

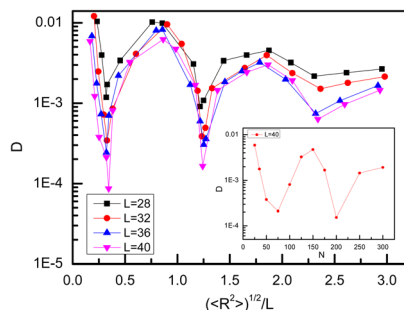


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Dynamics of polymer chains confined to a periodic cylinder: molecular dynamics simulation vs. Lifson–Jackson formula

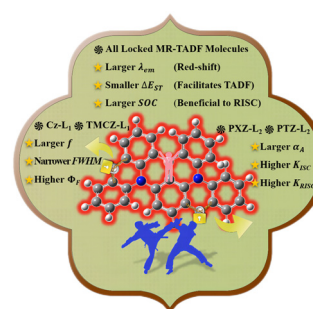
Jiaxin Wu, Zhiyong Yang, Xiaou Cai and Linxi Zhang*



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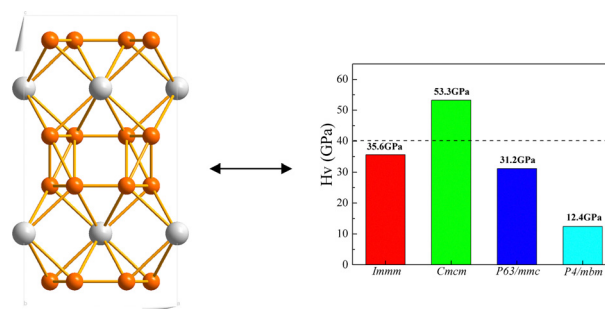
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Theoretical prediction of the structure and hardness of TiB₄ tetraborides from first-principles calculations

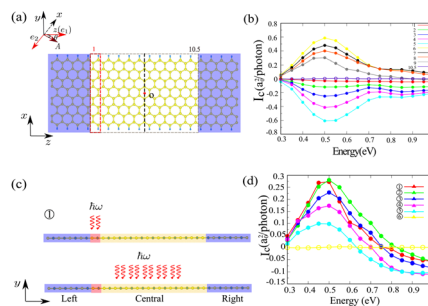
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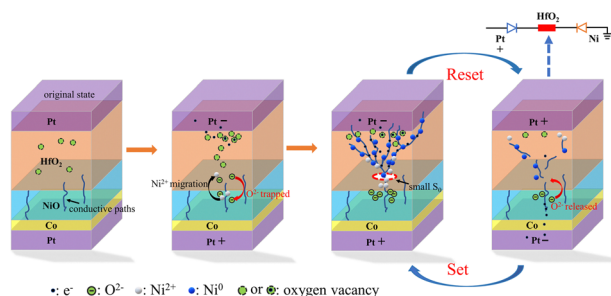
The effect of light-irradiated area on the spin dependent photocurrent in zigzag graphene nanoribbon junctions

Yuejun Li, Xiaofei Shang, Yan-Hong Zhou* and Xiaohong Zheng*



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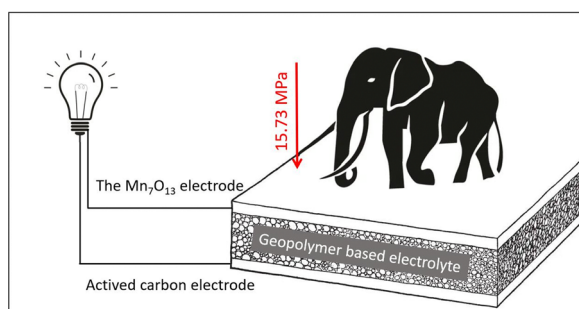
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Improved resistive switching performance and realized electric control of exchange bias in a NiO/HfO₂ bilayer structure

Yu Lu, Yuan Yuan, Ruobai Liu, Tianyu Liu, Jiarui Chen, Lujun Wei, Di Wu, Wei Zhang, Biao You and Jun Du*

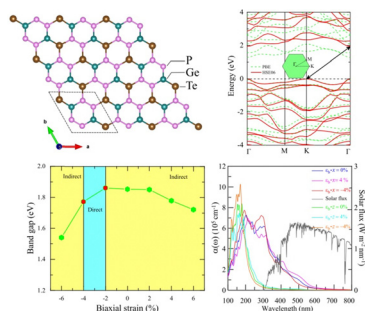
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A geopolymer membrane for application in a structural mechanics and energy storage difunctional supercapacitor

Jing-Lei Yang, Wei-Bin Zhang,* Shan-Shan Chai, Myat Myintzu Theint, Yi Yin, Ze-Qin Yang, Jia-Jun Li, Yu-Hui Yi and Xue-Jing Ma*

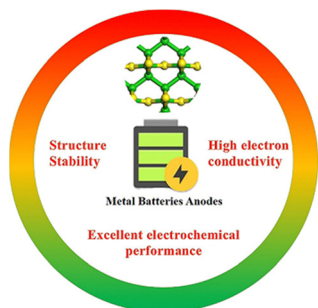
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Monolayer Ge₂Te₂P₄ as a promising photocatalyst for solar driven water-splitting: a DFT study

Trung D. Pham* and Tong D. Hien*

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B₃S₂ monolayer as an anode material for Na/K-ion batteries: a first-principles study

Danhong Wang, Zhifang Yang, Wenliang Li* and Jingping Zhang*

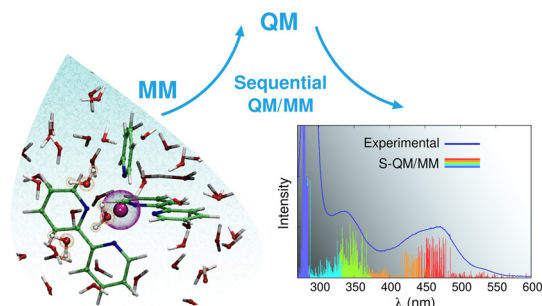


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Theoretical investigation of solvent and oxidation/deprotonation effects on the electronic structure of a mononuclear Ru-aqua-polypyridine complex in aqueous solution

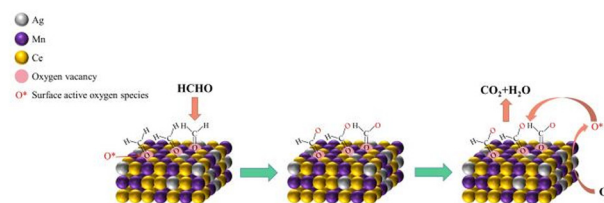
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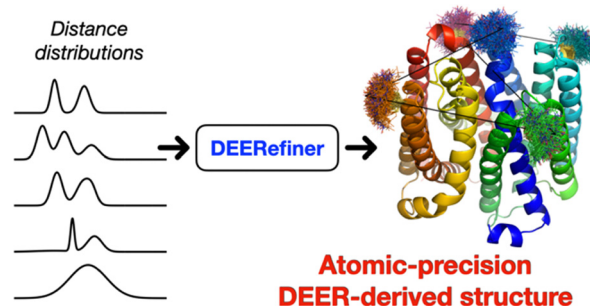
Chaomin Duan, Yanlin Zhou, Mianwu Meng,* Huang Huang,* Hua Ding, Qi Zhang, Renyuan Huang and Mengjuan Yan



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DEERefiner-assisted structural refinement using pulsed dipolar spectroscopy: a study on multidrug transporter LmrP

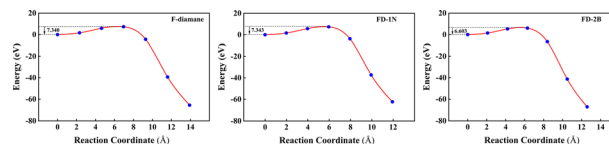
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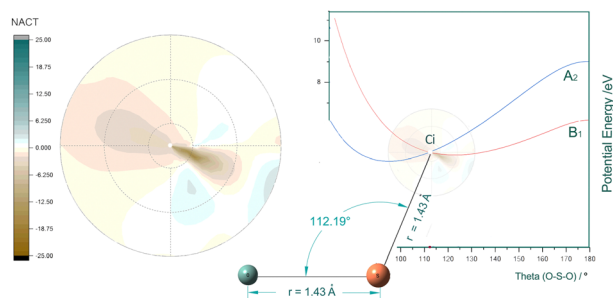
Structural stability and electronic and mechanical properties of nitrogen- and boron-doped fluorinated diamane

Lilin Gao, Yanning Liu, Yaqi Liang, Nan Gao,* Junsong Liu* and Hongdong Li*



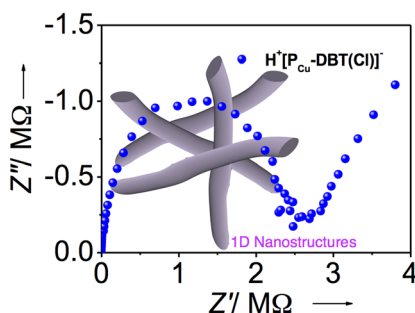
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Non-adiabatic coupling in the potential energy surfaces of SO_2 molecule

Sedigheh Pourestarabadi and Maryam Dehestani*

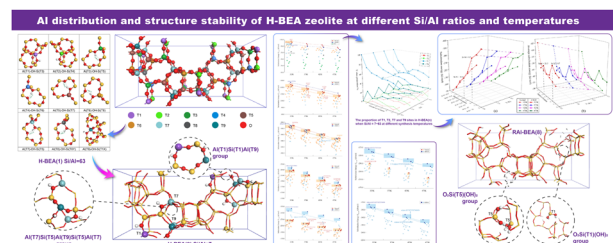
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Conducting 1D nanostructures from light-stimulated copper-metallated porphyrin-dibenzothiophene

Yelukala Ramakrishna, Madarapu Naresh, Botta Bhavani and Seelam Prasanthkumar*

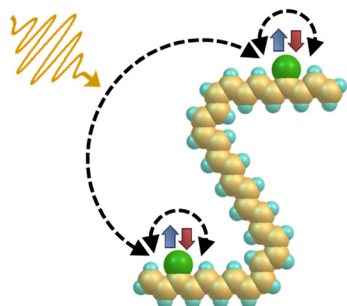
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Al distribution and structural stability of H-BEA zeolites at different Si/Al ratios and temperatures: a first-principles study

Changdong Li, Xiuqin Dong, Haipeng Yu and Yingzhe Yu*

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Laser-induced ultrafast spin-transfer processes in non-linear zigzag carbon chain systems

Mohamed Barhoumi, Jing Liu, Georgios Lefkidis* and Wolfgang Hübner

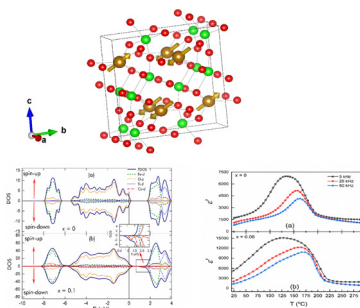


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Experimental and computational study on the influence of cobalt substitution on the structural, impedance, electronic, magnetic, and optical properties of pseudobrookite-structured Fe_2TiO_5

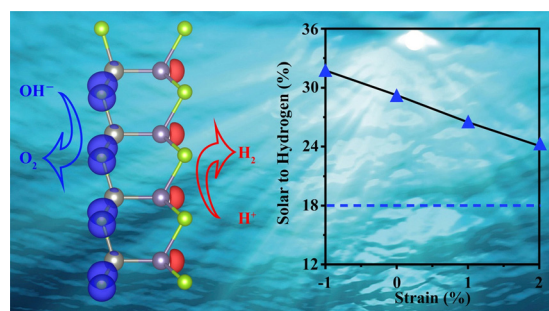
M. Naveed-Ul-Haq,* Anum Shafiq, Layiq Zia and Arif Mumtaz



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ZnGeSe_2 monolayer: water-splitting photocatalyst with ultrahigh solar conversion efficiency

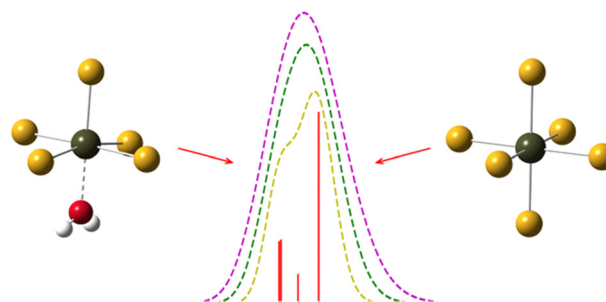
Guoting Nan, Wei Zhang, Xiaojun Yan, Xi Qin, Song Wu, Rufe Tang, Ming-Xia Tang, Lei Hu,* Lili Liu, Shifa Wang, Yuming Feng* and Wencai Yi*



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Excited states of polonium(IV): electron correlation and spin-orbit coupling in the Po^{4+} free ion and in the bare and solvated $[\text{PoCl}_5]^-$ and $[\text{PoCl}_6]^{2-}$ complexes

Nadiya Zhutova, Florent Réal, Eric Renault, Valérie Vallet* and Rémi Maurice*



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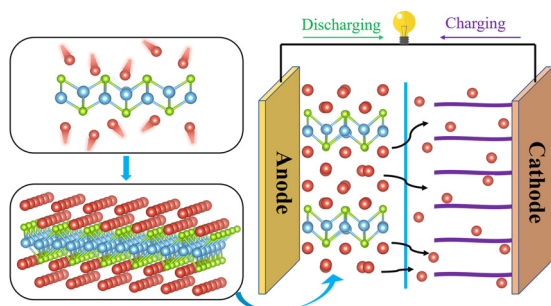
Waste dry cell derived photo-reduced graphene oxide and polyoxometalate composite for solid-state supercapacitor applications

Sukanya Maity, Bhimaraya R Biradar, Saurabh Srivastava, Pranay R. Chandewar, Debaprasad Shee, Partha Pratim Das* and Sib Sankar Mal*



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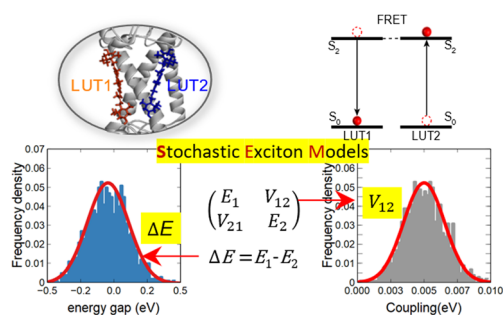
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A TiSe monolayer as a superior anode for applications of Li/Na/K-ion batteries

Mengke Wang, Shan Wang, Yunye Liang, Yiqun Xie, Xiang Ye* and Shoutian Sun*

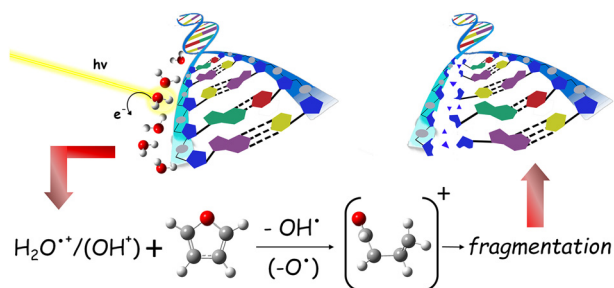
24636



Intermolecular resonance energy transfer between two lutein pigments in light-harvesting complex II studied by frenkel exciton models

Jiarui Li, Tao Zeng, Yu Zhai, Zexing Qu* and Hui Li*

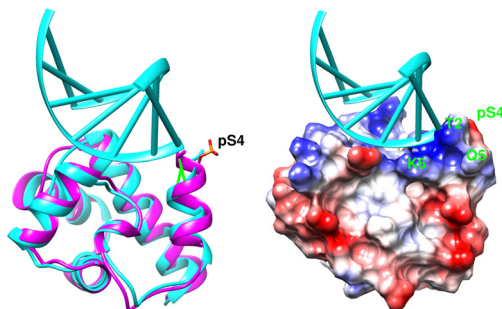
24643



H₂O⁺ and OH⁺ reactivity *versus* furan: experimental low energy absolute cross sections for modeling radiation damage

Daniela Ascenzi, Ewa Erdmann, Paola Bolognesi, Lorenzo Avaldi, Mattea Carmen Castrovilli, Roland Thissen, Claire Romanzin, Christian Alcaraz, Ismanuel Rabadan, Luis Mendez, Sergio Diaz-Tendero* and Antonella Cartoni*

24657



Mono-phosphorylation at Ser4 of barrier-to-autointegration factor (Banf1) significantly reduces its DNA binding capability by inducing critical changes in its local conformation and DNA binding surface

Ming Tang,* Amila Suraweera, Xuqiang Nie, Zilin Li, Pinglin Lai, James W. Wells, Kenneth J. O'Byrne, Robert J Woods, Emma Bolderson* and Derek J Richard*

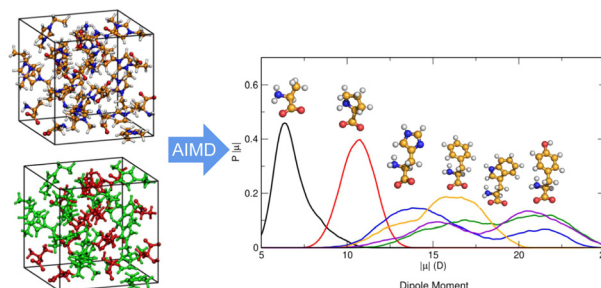


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24678

Locality in amino-acid based imidazolium ionic liquids

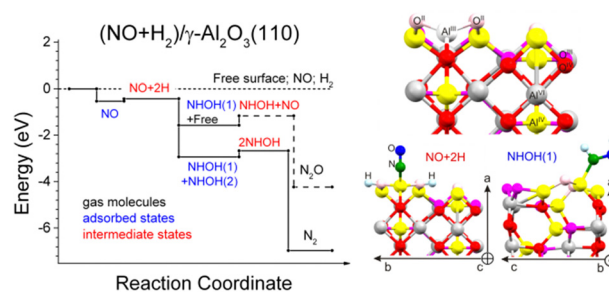
Wenbo Dong, Vahideh Alizadeh, Jan Blasius, Luke Wylie, Leonard Dick, Zhijie Fan and Barbara Kirchner*



24686

Catalytic activity of γ - $\text{Al}_2\text{O}_3(110)$ in the $\text{NO} + \text{H}_2$ reaction: a DFT study

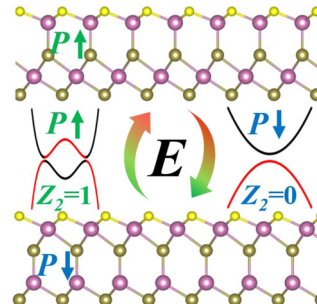
Alexander Cholach



24696

Non-volatile control of topological phase transition in an asymmetric ferroelectric $\text{In}_2\text{Te}_2\text{S}$ monolayer

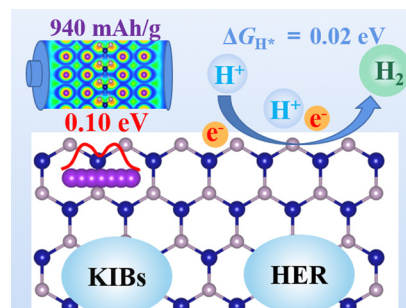
Guang Song,* Yangyang Wu, Lei Cao, Guannan Li, Bingwen Zhang, Feng Liang and Benling Gao



24705

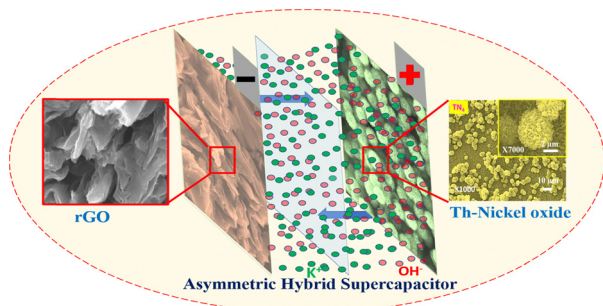
Metallic CrP_2 monolayer: potential applications in energy storage and conversion

Jiayu Gao, Wenyan Zhang, Xu Yan, Xiaohua Zhang, Sheng Wang and Guochun Yang*



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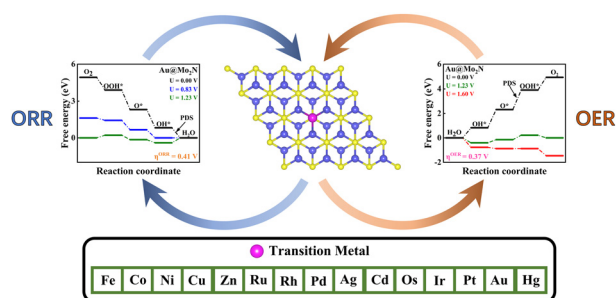
24712



Porous 3D columnar-sphere of NiO nanomaterials synthesized for supercapacitors *via* hydrothermal route: impact of thiourea concentration

Amar L. Jadhav, Sharad L. Jadhav, Bhalchandra K. Mandlekar and Anamika V. Kadam*

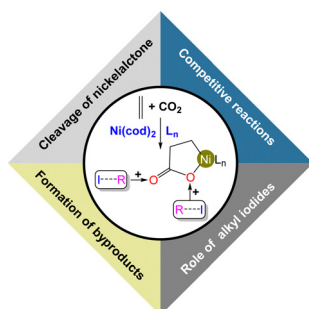
24721



Theoretical study of Mo₂N supported transition metal single-atom catalyst for OER/ORR bifunctional electrocatalysis

Long Lin, Xiaoqin Long, Xinyu Yang, Pei Shi and Linlin Su*

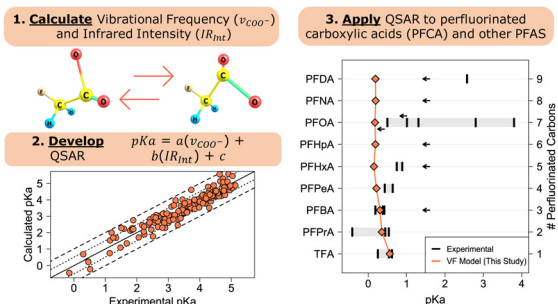
24733



Mechanistic study on the formation of the alkyl acrylates from CO₂, ethylene and alkyl iodides over nickel-based catalyst

Youcai Zhu, Yue Mu, Li Sun, Zuoxiang Zeng and Zhen Liu*

24745



pK_a prediction of per- and polyfluoroalkyl acids in water using *in silico* gas phase stretching vibrational frequencies and infrared intensities

Jimmy Murillo-Gelvez, Olga Dmitrenko, Tiffany L. Torralba-Sanchez, Paul G. Tratnyek and Dominic M. Di Toro*

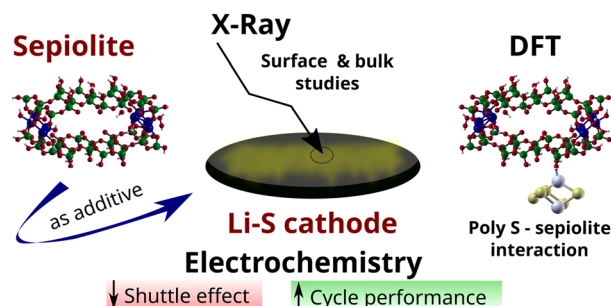


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24761

Sepiolite as a novel polysulfide trapper for energy applications: an electrochemical, X-ray spectroscopic and DFT study

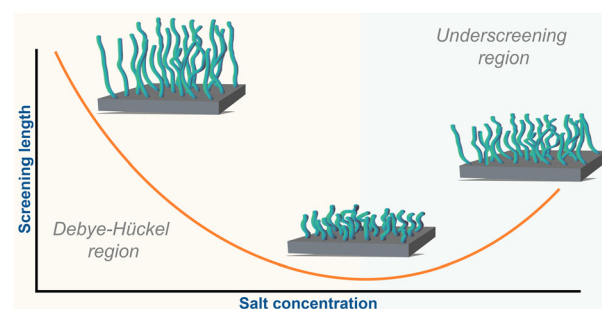
Francisco Javier García-Soriano,* Sergio Andrés Ceppi, Fernando Pablo Cometto, Emiliano Nicolás Primo, Daniel Eugenio Barraco, Ezequiel Pedro Marcos Leiva, Guillermina Leticia Luque, Guillermo Stutz, German Lener* and Maria Victoria Bracamonte*



24770

Underscreening in concentrated electrolytes: re-entrant swelling in polyelectrolyte brushes

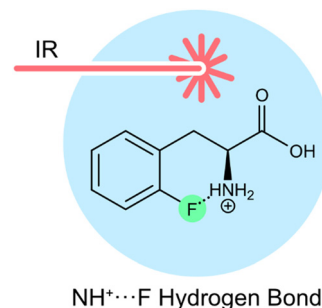
Hayden Robertson, Gareth R. Elliott, Andrew R. J. Nelson, Anton P. Le Brun, Grant B. Webber, Stuart W. Prescott, Vincent S. J. Craig, Erica J. Wanless and Joshua D. Willott*



24783

Cryogenic infrared spectroscopy reveals remarkably short $\text{NH}^+ \cdots \text{F}$ hydrogen bonds in fluorinated phenylalanines

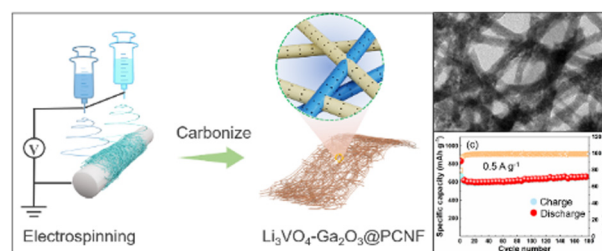
Marc Safferthal, Kim Greis, Rayoon Chang, Carla Kirschbaum, Waldemar Hoffmann, Gerard Meijer, Gert von Helden and Kevin Pagel*



24789

Heterostructured $\text{Li}_3\text{VO}_4\text{-Ga}_2\text{O}_3$ -embedded porous carbon nanofibers as advanced anode materials for lithium-ion batteries

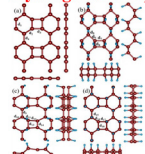
Canyang Chen, Cunyuan Pei,* Song Yang, Huijuan Ma, Dongmei Zhang, Bing Sun and Shibing Ni*



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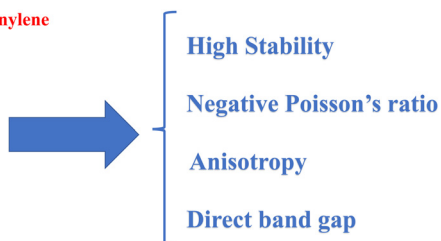
24797

Hydrogenated biphenylene



$$i\hbar \frac{\partial}{\partial t} |\Psi\rangle = \hat{H} |\Psi\rangle$$

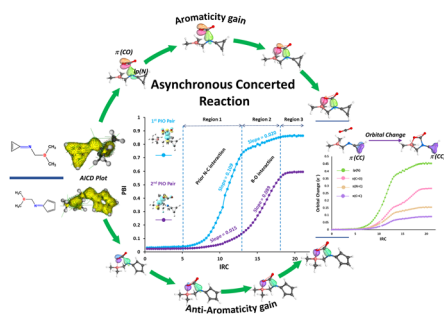
DFT (VASP)



Structural, mechanical, electronic and optical properties of biphenylene hydrogenation: a first-principles study

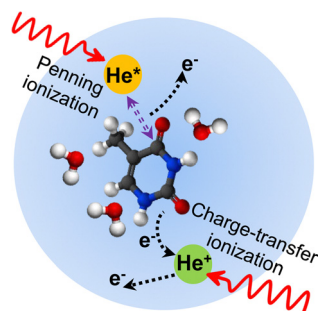
Kai Chen, Jian Zhou, Wuyan Zhao, Riyi Yang, Chong Qiao, Wan-Sheng Su,* Yuxiang Zheng, Rongjun Zhang, Liangyao Chen and Songyou Wang*

24809

PIO and IBO analysis to unravel the hidden details of the CO₂ sequestration mechanism of aromatically tempered N/B-based IFLPs

Mohmmad Faizan, Adarsh Kumar, Mucherla Raghasudha and Ravinder Pawar*

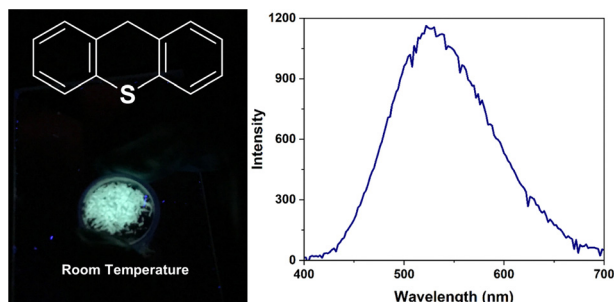
24819



Secondary ionization of pyrimidine nucleobases and their microhydrated derivatives in helium nanodroplets

Jakob D. Asmussen, Abdul R. Abid, Akgash Sundaralingam, Björn Bastian, Keshav Sishodia, Subhendu De, Ltaief Ben Ltaief, Sivarama Krishnan, Henrik B. Pedersen and Marcel Mudrich*

24829



Photophysical investigation into room-temperature emission from xanthene derivatives

Kristen Harrington, David T. Hogan, Todd C. Sutherland* and Kevin Stamplecoskie*

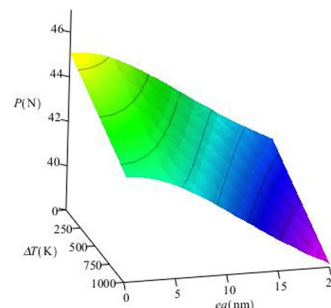


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24838

A nonlocal strain gradient shell model with the surface effect for buckling analysis of a magneto-electro-thermo-elastic cylindrical nanoshell subjected to axial load

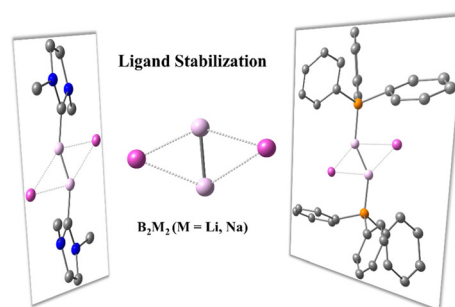
Yifei Gui and Zhisong Li*



24853

Mimicking the C₂ molecule: M₂B₂ and M₃B₂⁺ clusters (M = Li, Na) and the reactivity of the N-heterocyclic carbene bound Li₂B₂ complex

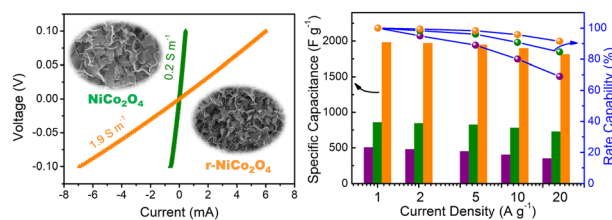
Yu-qian Liu, Gai-ru Yan, Li-juan Cui, Bing Yan, Sudip Pan* and Zhong-hua Cui*



24862

Oxygen defect-mediated NiCo₂O₄ nanosheets as the electrode for pseudocapacitors with improved rate capability

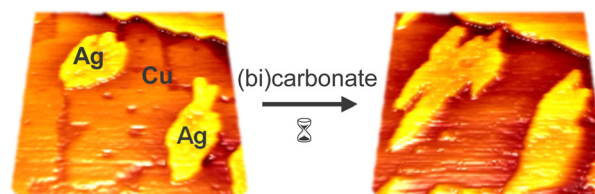
Wen You, Mengyuan Li, Qiong Li, Jizhou Jiang, Kun Xiang* and Mingjiang Xie*



24871

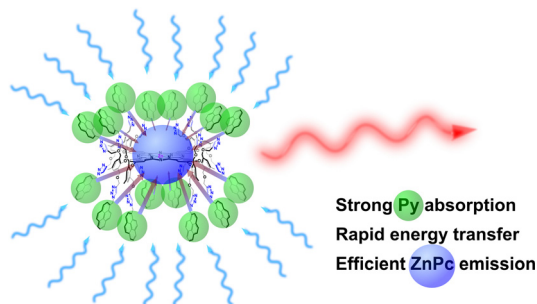
In situ scanning tunneling microscopy studies of carbonate-induced restructuring of Ag-decorated Cu(100) electrodes

Reihaneh Amirbeigi-arab and Olaf M. Magnussen*



RESEARCH PAPERS

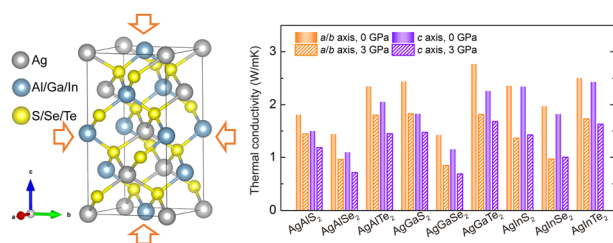
24878



Covalently linked pyrene antennas for optically dense yet aggregation-resistant light-harvesting systems

Lubna Salah, Saad Makhseed, Basma Ghazal, Ahmed Abdel Nazeer, Marc K. Etherington, Carlito S. Ponseca Jr., Chunyong Li, Andrew P. Monkman, Andrew Danos* and Ali Shuaib*

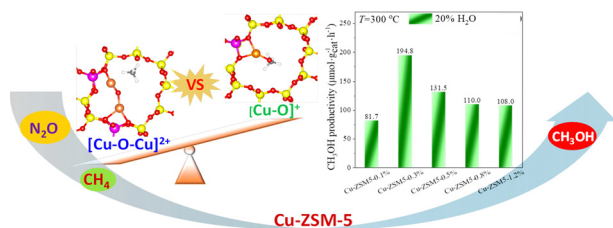
24883



Soft phonon modes lead to suppressed thermal conductivity in Ag-based chalcopyrites under high pressure

Kunpeng Yuan, Xiaoliang Zhang,* Yufei Gao and Dawei Tang*

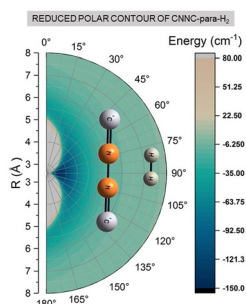
24894



Mechanistic insight into the effect of active site motif structures on direct oxidation of methane to methanol over Cu-ZSM-5

Chengna Dai, Yuchan Zhang, Ning Liu,* Gangqiang Yu, Ning Wang, Ruinian Xu and Biaohua Chen

24904



New potential energy surface and rotational deexcitation cross-sections of CNNC by *para*-H₂ (*j_p* = 0)

Ritika and T. J. Dhillip Kumar*

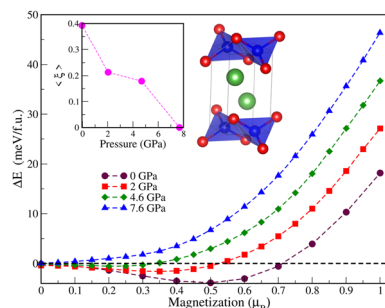


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24912

Proximity of superconducting LaCoSi to a ferromagnetic quantum critical point

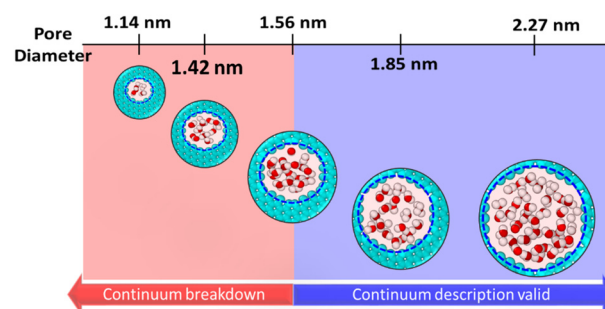
Himanshu and J. J. Pulikkotil*



24919

The validity of the continuum modeling limit in a single pore flows to the molecular scale

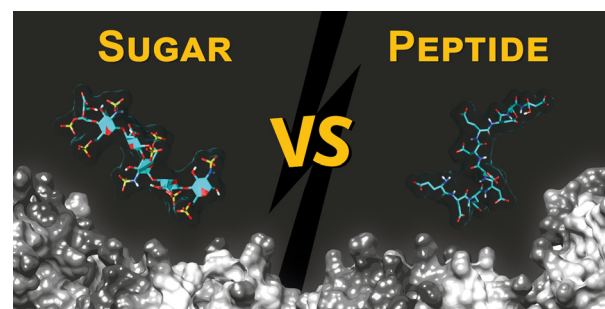
Jaber Al Hossain and BoHung Kim*



24930

Ligand binding of interleukin-8: a comparison of glycosaminoglycans and acidic peptides

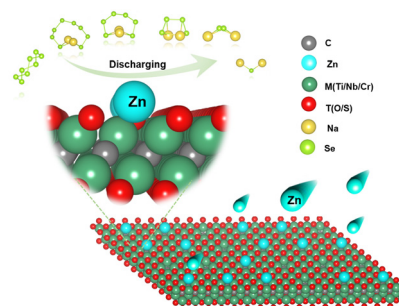
Christian Schulze, Annemarie Danielsson, Adam Liwo, Daniel Huster, Sergey A. Samsonov* and Anja Penk*



24948

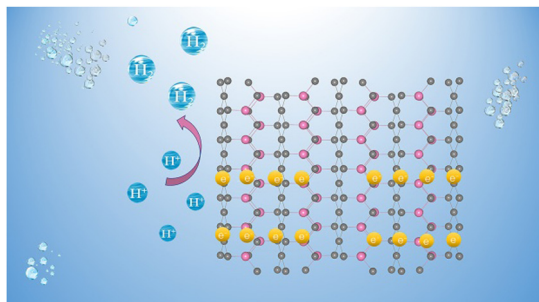
Rational design of MXene-based single atom catalysts for Na–Se batteries from sabatier principle

Chunlei Wei, MengMeng Ge, Timing Fang,* Xiao Tang and Xiaomin Liu*



RESEARCH PAPERS

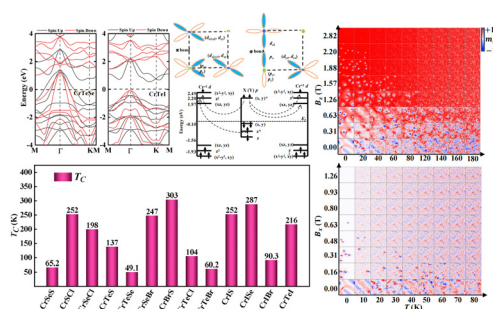
24960



Photocatalytic water splitting for hydrogen production with high efficiency monolayer In_2Te_5 : a theoretical study

Cong Zhang, Meiping Tan, Xin Lu, Wenzhuo Li, Yang Yu, Qiang Wang, Wenjun Zhang, Xiaole Qiu and Hongchao Yang*

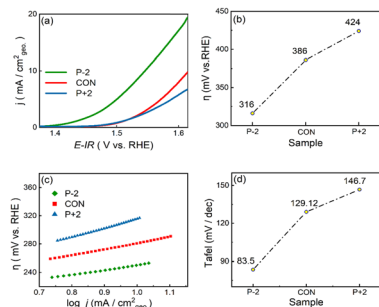
24968



Electronic properties, skyrmions and bimerons in Janus CrXY ($X, Y = \text{S, Se, Te, Cl, Br, I}$, and $X \neq Y$) monolayers

Zhihao Guan, Zhong Shen, Yufei Xue, Tingting Zhong, Xiaoping Wu and Changsheng Song*

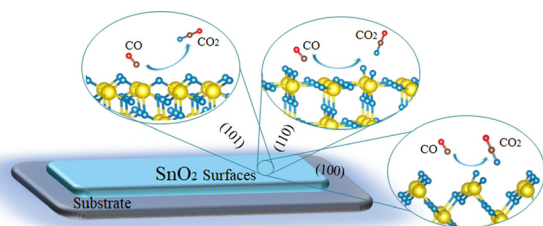
24976



Modulating the oxygen evolution reaction activity of $\text{SrIrO}_3/\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})_{0.7}\text{Ti}_{0.3}\text{O}_3$ catalysts using electric-field polarization

Anxin Meng, Jiabao Ding, Caiqin Luo, Mian Qin* and Weifeng Zhang*

24985



Preferred surface orientation for CO oxidation on SnO_2 surfaces

Zineb Kerrami*, Anass Sibari, Mohammed Benaissa and Abdelkader Kara*

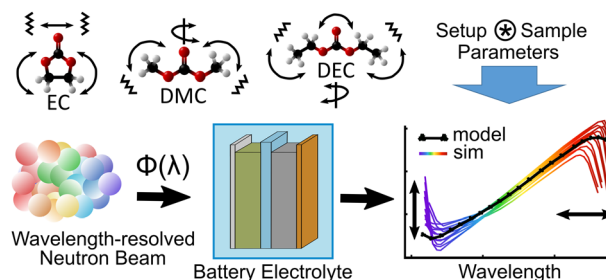


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24993

Prospects of spectroscopic neutron imaging: optimizing experimental setups in battery electrolyte research

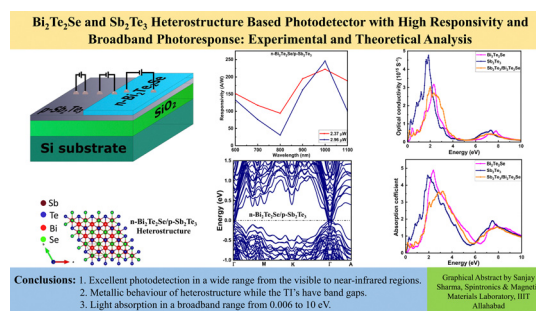
E. Ricardo Carreón Ruiz, Natalie Stalder, Jongmin Lee, Lorenz Gubler and Pierre Boillat*



25008

Bi₂Te₂Se and Sb₂Te₃ heterostructure based photodetectors with high responsivity and broadband photoresponse: experimental and theoretical analysis

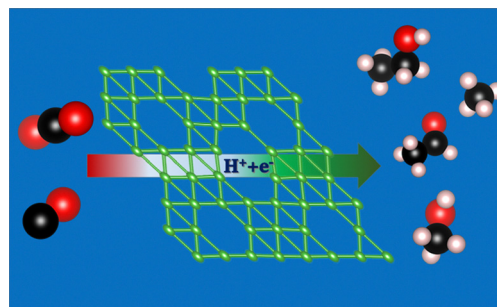
Sandeep Kumar Verma, Sanjay Sharma, Gyanendra Kumar Maurya, Vidushi Gautam, Roshani Singh, Ajeet Singh, Kavindra Kandpal, Pramod Kumar,* Arun Kumar and Claudia Wiemer*



25018

Single B-vacancy enriched α_1 -borophene sheet: an efficient metal-free electrocatalyst for CO₂ reduction

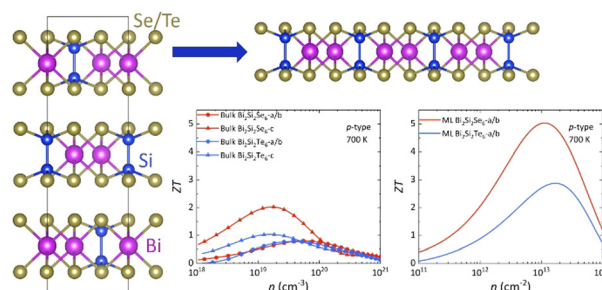
Prodyut Roy, Sourav Ghoshal, Anup Pramanik and Pranab Sarkar*



25029

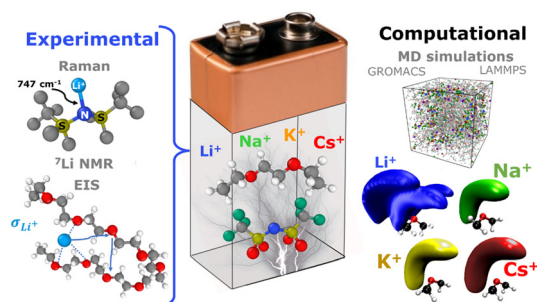
Dimensionality reduction induced synergetic optimization of the thermoelectric properties in Bi₂Si₂X₆ (X = Se, Te) monolayers

Tingting Zhang, Suiting Ning, Ziyi Zhang, Ning Qi and Zhiqian Chen*



RESEARCH PAPERS

25038



Synergistic theoretical and experimental study on the ion dynamics of bis(trifluoromethanesulfonyl)-imide-based alkali metal salts for solid polymer electrolytes

Brigette Althea Fortuin, Jon Otegi,
 Juan Miguel López del Amo,
 Sergio Rodríguez Peña, Leire Meabe, Hegoi Manzano,*
 María Martínez-Ibañez* and Javier Carrasco*

CORRECTION

25055

Correction: Lone pair driven anisotropy in antimony chalcogenide semiconductors

Xinwei Wang, Zhenzhu Li, Seán R. Kavanagh, Alex M. Ganose and Aron Walsh*

