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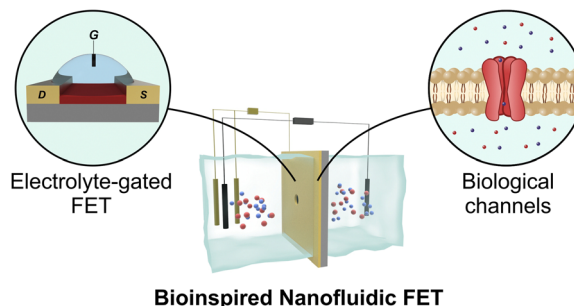
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REVIEWS

10471

Advances in nanofluidic field-effect transistors: external voltage-controlled solid-state nanochannels for stimulus-responsive ion transport and beyond

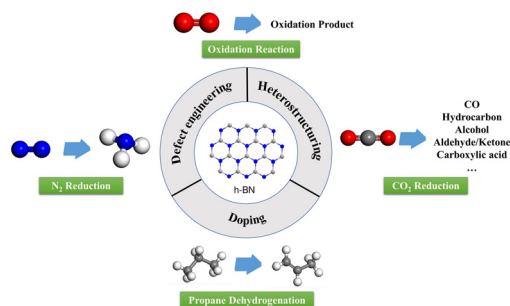
G. Laucirica,* Y. Toun-Terrones, V. M. Cayón,
M. E. Toimil-Molares, O. Azzaroni and W. A. Marmisollé*



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Adsorption and activation of small molecules on boron nitride catalysts

Baiyu Miao, Zhihuan Qiu, Ziheng Zhen, Youwei Yang,
Zhibo Yang, Tiantian Xiao, Jing Lv, Shouying Huang,
Yue Wang* and Xinbin Ma



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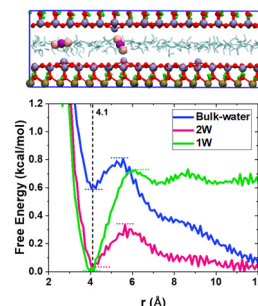


COMMUNICATIONS

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Confinement-induced clustering of H₂ and CO₂ gas molecules in hydrated nanopores

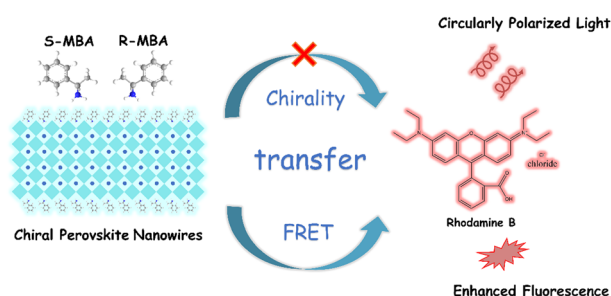
Aditya Choudhary and Tuan A. Ho*



10515

Discriminatory fluorescence and FRET in the chiral-perovskite/RhB system

Hongxu Li, Ying Cui, Min Tao, Shuo Sun, Xinyao Yan and Yin Xiao*

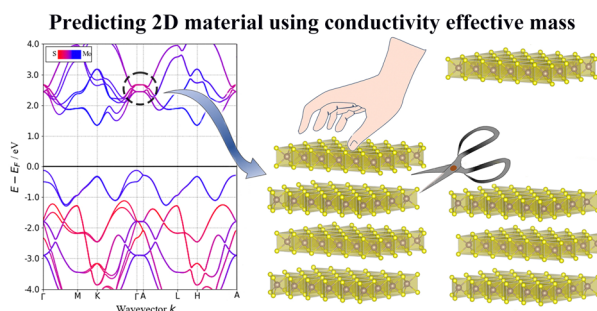


RESEARCH PAPERS

10520

Predicting two-dimensional semiconductors using conductivity effective mass

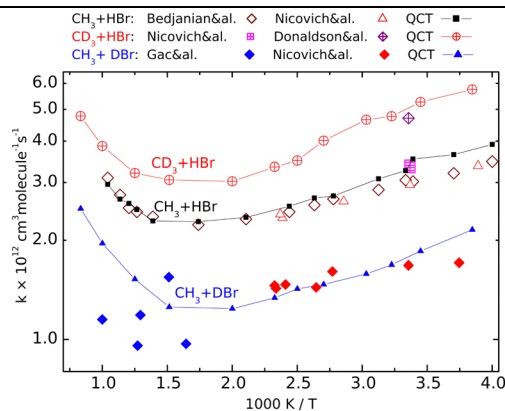
Wenjun Zhang, Zhikun Yao and Lee A. Burton*



10530

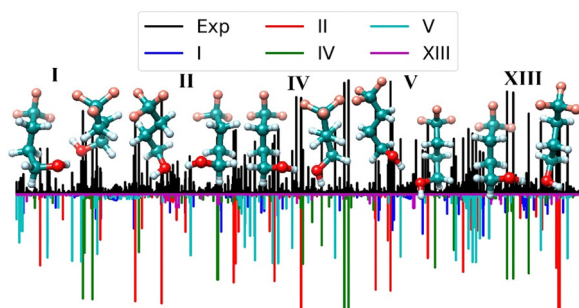
Theoretical dynamics studies of the CH₃ + HBr → CH₄ + Br reaction: effects of isotope substitution and vibrational excitation of CH₃

Péter Szabó* and György Lendvay*



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Binary conformers of a flexible, long-chain fluoroalcohol: dispersion controlled selectivity and relative abundances in a jet

Tao Lu, Fan Xie, Nathan A. Seifert, Reihaneh Hamidi Mejlaj, Wolfgang Jäger and Yunjie Xu*

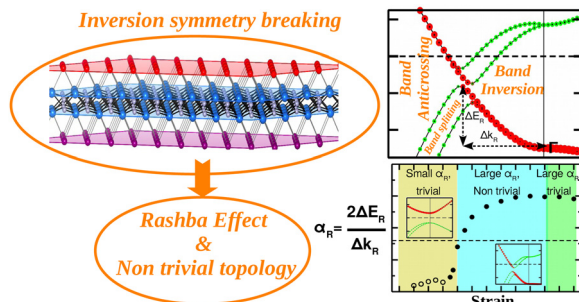
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Effect of trimethylamine-*N*-oxide on the phase separation of aqueous polyethylene glycol-600-Dextran-75 two-phase systems

Amber R. Titus, Patrick Herron, Kiril A. Streletsky, Pedro P. Madeira, Vladimir N. Uversky and Boris Y. Zaslavsky*

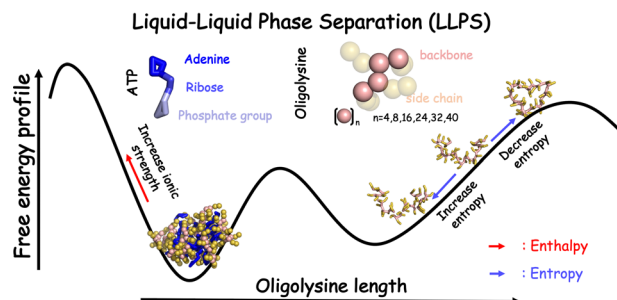
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First principles predictions of structural, electronic and topological properties of two-dimensional Janus $\text{Ti}_2\text{N}_2\text{XI}$ ($\text{X} = \text{Br}, \text{Cl}$) structures

Shiladitya Karmakar, Soumendu Datta and Tanusri Saha-Dasgupta*

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Understanding and fine tuning the propensity of ATP-driven liquid-liquid phase separation with oligolysine

Qiang Zhu, Yongxian Wu and Ray Luo*

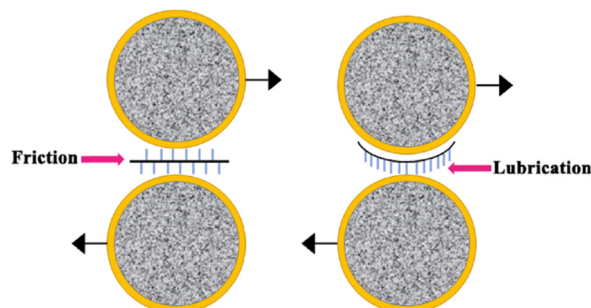


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The mechanism of fluidity improvement of cement slurry by graphene oxide: a study on nanofriction

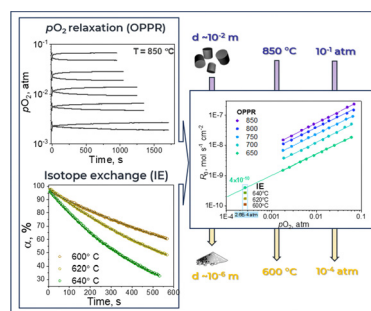
Xiang Ji, Dongshuai Hou, Muhan Wang, Liu Qing, Fen Hong, Yanshuai Wang, Guohao Fang, Shuxian Hong and Mengmeng Li*



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Consistent interpretation of isotope and chemical oxygen exchange relaxation kinetics in $\text{SrFe}_{0.85}\text{Mo}_{0.15}\text{O}_{3-\delta}$ ferrite

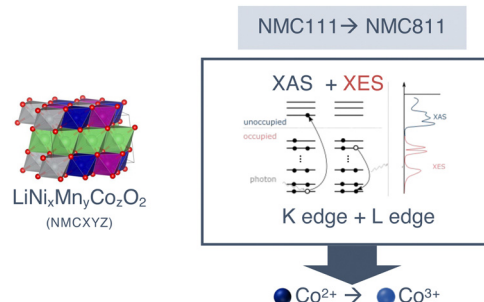
Marina Arapova,* Stanislav Chizhik, Olga Bragina, Rostislav Guskov, Vladimir Sobolev and Alexander Nemudry



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A multi-edge study: investigating Co oxidation states of pristine $\text{LiNi}_x\text{Mn}_y\text{Co}_{1-x-y}\text{O}_2$ cathode materials by high energy-resolution X-ray spectrometry

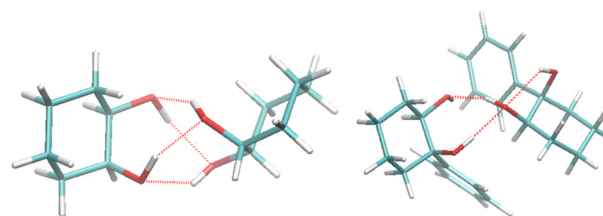
Karina Bzheumikhova,* Claudia Zech, Kai Schüller, John Vinson, Yves Kayser and Burkhard Beckhoff



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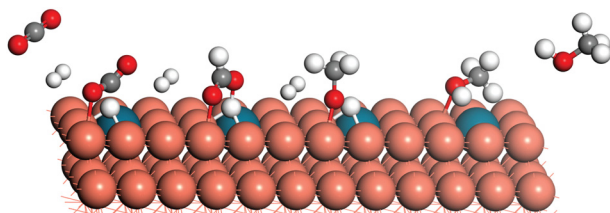
Homochiral vs. heterochiral preference in chiral self-recognition of cyclic diols

Jennifer Dupont, Beppo Hartwig, Katia Le Barbu-Debus, Valeria Lepere, Regis Guillot, Martin A. Suhm and Anne Zehnacker*



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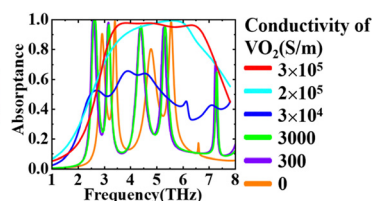
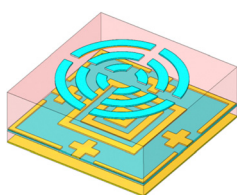
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A microkinetic study of CO₂ hydrogenation to methanol on Pd₁-Cu(111) and Pd₁-Ag(111) catalysts: a DFT analysis

Abdulrauf Onimisi Ibrahim,* Wan Mohd Ashri Wan Daud,*
Muhamad Fazly Abdul Patah,* Ahmed Halilu,
Joon Ching Juan* and Gazali Tanimu

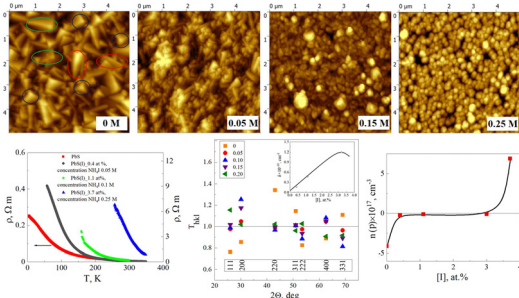
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A dual functional tunable terahertz metamaterial absorber based on vanadium dioxide

Junhao Niu, Qiang Hui, Wei Mo, Qianyu Yao,
Haozhuo Gong, Renfang Tian and Aijun Zhu*

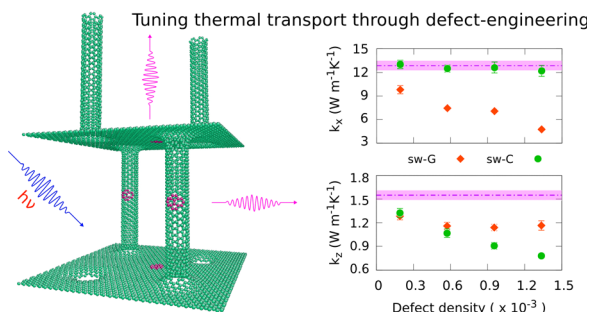
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Charge carrier transport in PbS films doped with iodine

L. N. Maskaeva,* A. V. Pozdin, A. Yu. Pavlova,
Yu. V. Korkh, T. V. Kuznetsova, V. I. Voronin,
K. E. Krivonosova, T. B. Charikova and V. F. Markov

10650



Thermal transport in a defective pillared graphene network: insights from equilibrium molecular dynamics simulation

Vivekkumar Panneerselvam and Sarith P Sathian*



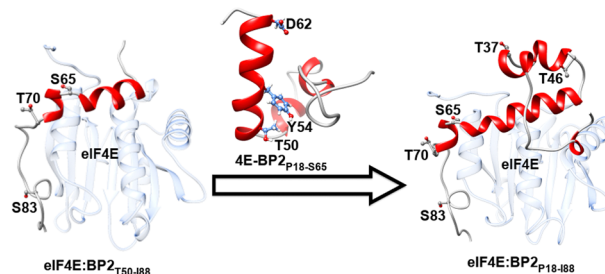
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The human eIF4E:4E-BP2 complex structure for studying hyperphosphorylation

Juan Zeng,* CuiMin Lu, Xuan Huang and Yang Li*

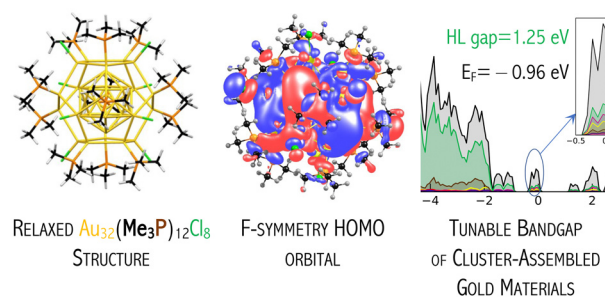
The human eIF4E:4E-BP2 complex includes all five reported phosphorylation sites.



10673

Tuning the electronic structure of gold cluster-assembled materials by altering organophosphine ligands

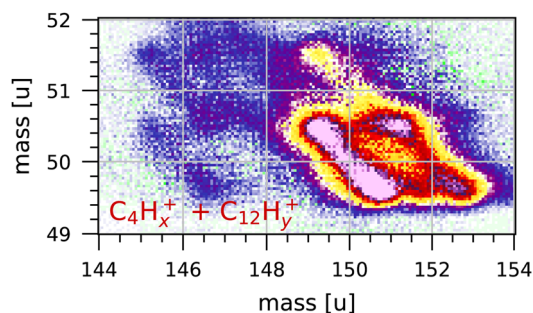
Celina Sikorska,* Emma Vincent, Andreas Schnepf and Nicola Gaston



10688

Coincidence mass spectrometry study of double ionization of pyrene by 70 eV electron impact

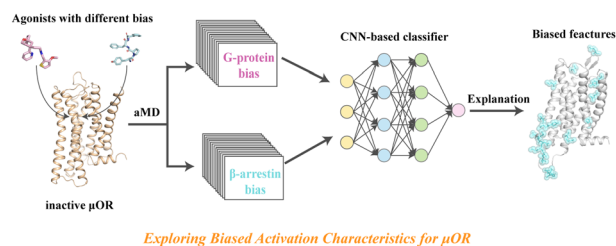
Peter J. M. van der Burgt* and Marcin L. Gradziel



10698

Exploring biased activation characteristics by molecular dynamics simulation and machine learning for the μ -opioid receptor

Jianfang Chen, Qiaoling Gou, Xin Chen, Yuanpeng Song, Fuhui Zhang* and Xuemei Pu*

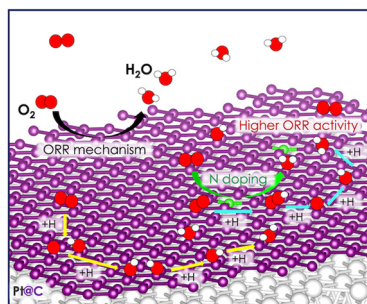


Exploring Biased Activation Characteristics for μ OR



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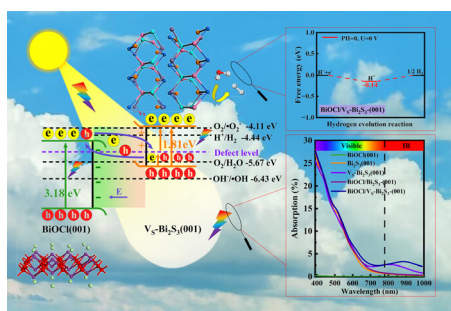
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First-principles studies of enhanced oxygen reduction reactions on graphene- and nitrogen-doped graphene-coated platinum surfaces

Ho Ngoc Nam,* Quan Manh Phung, Pongpol Choeichom, Yusuke Yamauchi and Nagahiro Saito*

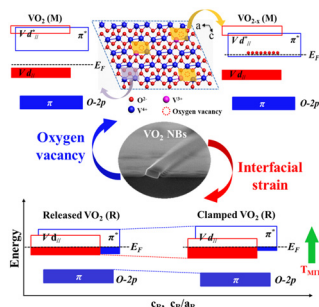
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The direct Z-scheme character and roles of S vacancy in BiOCl/Bi₂S₃-(001) heterostructures for superior photocatalytic activity: a hybrid density functional investigation

Wentao Wang,* Zuoyin Liu, Hongwei Nie and Bo Kong*

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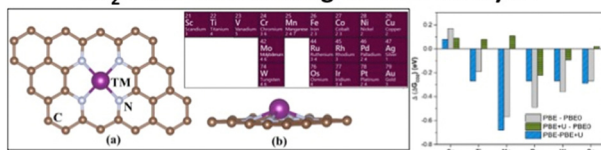


Effects of oxygen vacancies and interfacial strain on the metal–insulator transition of VO₂ nanobeams

Xitao Guo, Xin Liu, Zainab Zafar, Guiquan Cheng, Yunhai Li, Haiyan Nan, Lianghua Lin and Jijun Zou

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CO₂ Activation on Single-Atom Catalysts



CO₂ electroreduction on single atom catalysts: the role of the DFT functional

Debolina Misra, Giovanni Di Liberto* and Gianfranco Pacchioni

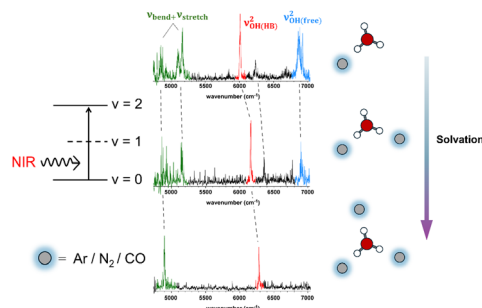


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Near-infrared spectroscopy of $\text{H}_3\text{O}^+ \cdots \text{X}_n$ ($\text{X} = \text{Ar}, \text{N}_2$, and CO , $n = 1-3$)

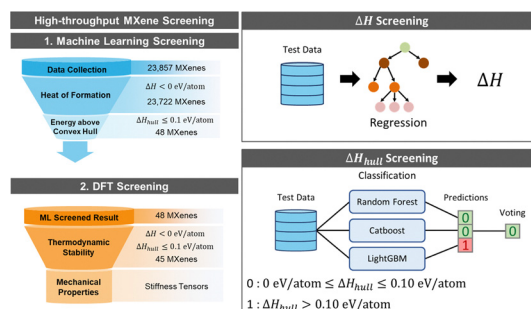
Qian-Rui Huang, Kazuyoshi Yano, Yaodi Yang,
Asuka Fujii* and Jer-Lai Kuo*



10769

Exploring the large chemical space in search of thermodynamically stable and mechanically robust MXenes *via* machine learning

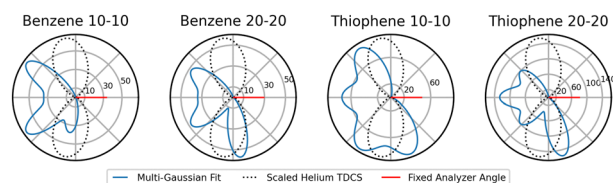
Jaejung Park, Minseon Kim, Heekyu Kim, Jaejun Lee,
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Seungchul Lee*



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Coincidence measurements of photodouble ionization of benzene and thiophene

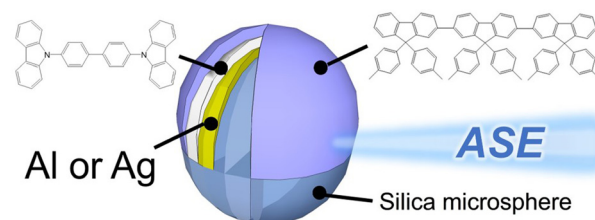
Nicholas L. Wong,* Jason Howard, Ben Delaney,
Emma Sokell, Paola Bolognesi and Lorenzo Avaldi



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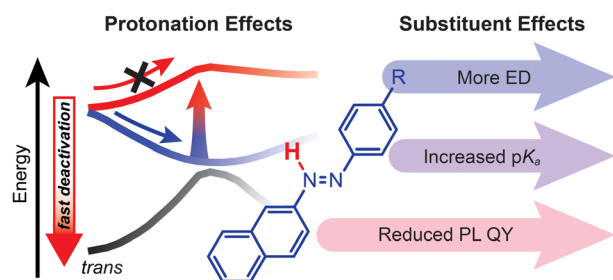
Suppression of the plasmon-quenching effect on light amplification in 20-μm-diameter plasmonic whispering gallery mode resonators fabricated from bowl-shaped organic/metal thin films

Minami Takaishi, Takeshi Komino,* Akihiro Kameda,
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Kazusuke Maenaka and Hiroyuki Tajima



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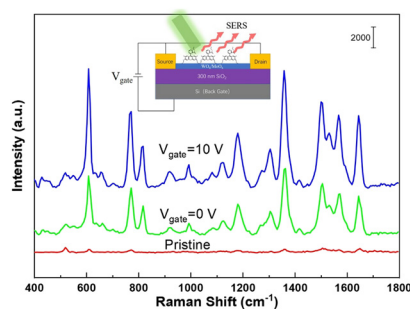
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Controlling excited-state dynamics via protonation of naphthalene-based azo dyes

Shea M. Martin, Robert C. Hamburger, Tao Huang, Lisa A. Fredin* and Elizabeth R. Young*

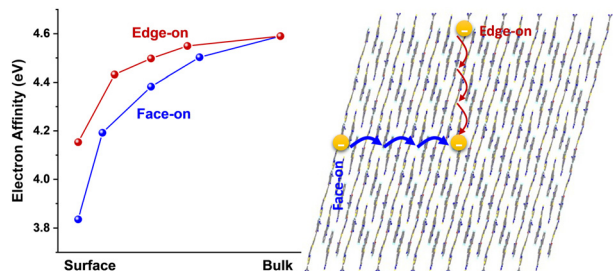
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A WO_x/MoO_x hybrid oxide based SERS FET and investigation on its tunable SERS performance

Kaibo Yuan, Qingin Qian, Miaomiao Wu, Bingxia Wang,* Shuweng Zeng, Dong Chen,* Muhammad Danang Birowosuto, Diing Shen Ang and Chenjie Gu*

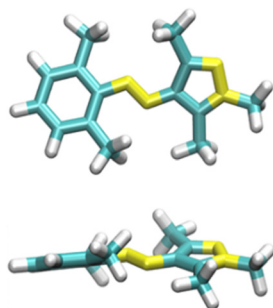
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The impact of molecular orientations on the energy levels of A–D–A acceptors: implications for the charge separation driving force of organic solar cells

Miaofei Huang, Guangchao Han and Yuanping Yi*

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Photoswitching of arylazopyrazoles upon S_1 ($n\pi^*$) excitation studied by transient absorption spectroscopy and *ab initio* molecular dynamics

Till Reichenauer, Marcus Böckmann, Katharina Ziegler, Vikas Kumar, Bart Jan Ravoo,* Nikos L. Doltsinis* and Sebastian Schlücker*

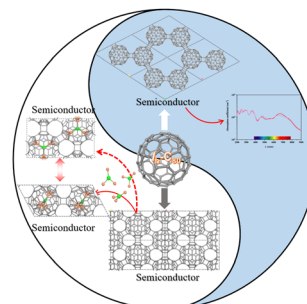


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Two-dimensional fullerene-based monolayer materials assembled by C_{80} and $Sc_3N@C_{80}$

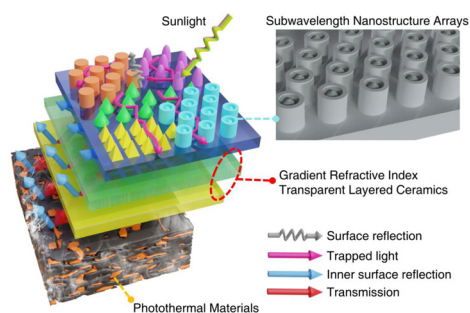
Yang Zhao, Yu Guo, Yanyan Zhao, Xueke Yu, Nikolai Cherenda, Yan Su* and Jijun Zhao*



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Modeling of the synergistic anti-reflection effect in gradient refractive index films integrated with subwavelength structures for photothermal conversion

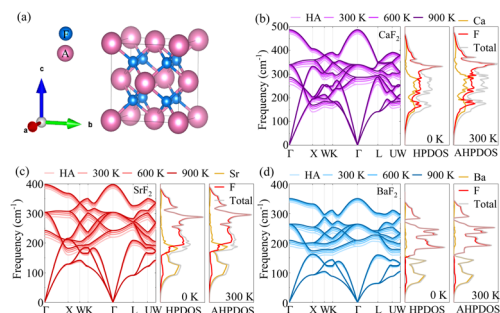
Yixuan Wang, Jingxu Shi, Xiangjun Liu, Bing Chen* and Xiangfu Wang*



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Study on lattice dynamics and thermal conductivity of fluorite AF_2 ($A = Ca, Sr, Ba$) based on first principles calculations

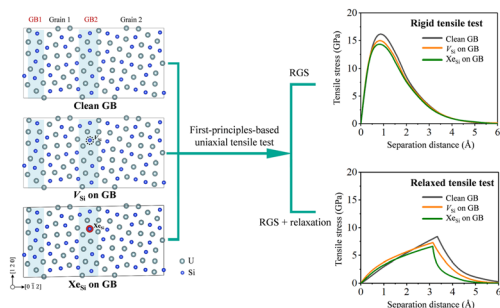
Peipei Liu, Yinchang Zhao,* Xichang Wang, Jun Ni and Zhenhong Dai*



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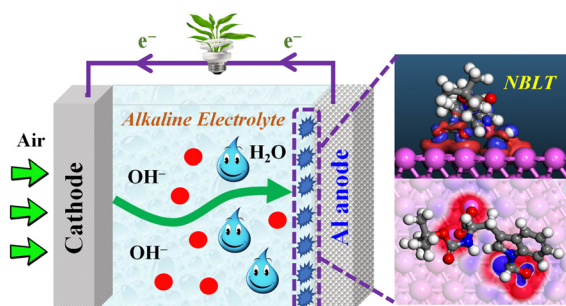
Effect of fission defects on tensile strength of U_3Si_2 $\Sigma 5(210)$ grain boundary from first-principles calculations

Jiajun Zhao, Dan Sun,* Liu Xi, Ping Chen, Jijun Zhao and Yuanyuan Wang*



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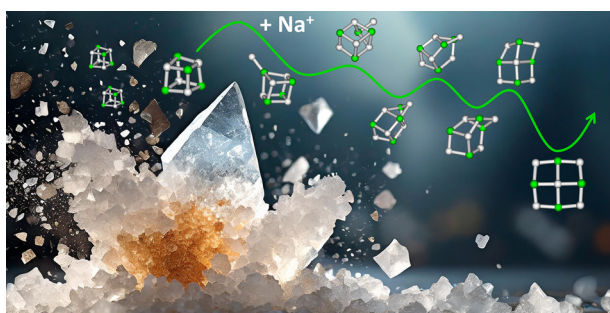
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Self-assembly of an amino acid derivative as an anode interface layer for advanced alkaline Al–air batteries

Lei Guo,* Lei Zhu, Yue Huang, Yan Tan, Alessandra Gilda Ritacca, Xingwen Zheng, Senlin Leng and Baoguo Wang

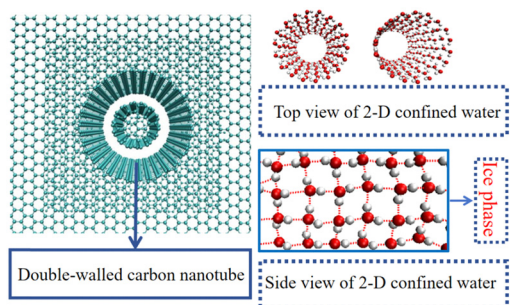
10904



Magic cluster sizes of cationic and anionic sodium chloride clusters explained by statistical modeling of the complete phase space

Jessica C. Hartmann, Sarah J. Madlener, Christian van der Linde, Milan Ončák* and Martin K. Beyer*

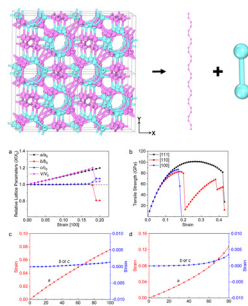
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Terahertz electric field induced melting and transport of monolayer water confined in double-walled carbon nanotubes

Yue Wu, Zi Wang, Shuang Li and Jiaye Su*

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Theoretical insights into the structural, mechanical, and electronic properties of bcc-C40 carbon

Ying Ma, Pan Ying,* Kun Luo, Yingju Wu, Baozhong Li and Julong He*

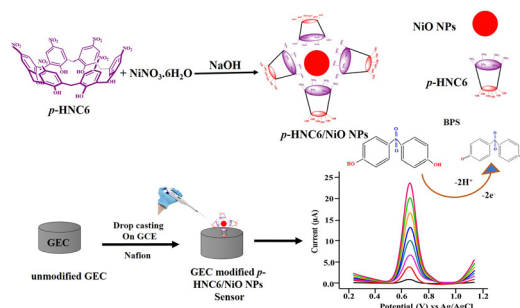


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A NiO-nanostructure-based electrochemical sensor functionalized with supramolecular structures for the ultra-sensitive detection of the endocrine disruptor bisphenol S in an aquatic environment

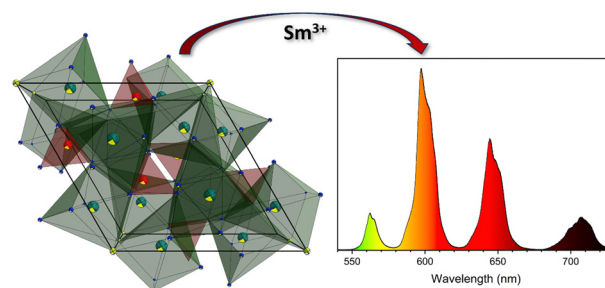
Ali Hyder, Akbar Ali, Jamil Ahmed Buledi, Roomia Memon, Bader S. Al-Anzi,* Ayaz Ali Memon,* Mohsin Kazi, Amber Rehana Solangi, Jun Yang* and Khalid Hussain Thebo*



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Characterization of Sm^{3+} -activated carbonated calcium chlorapatite phosphors for theranostic applications: a comparative study of co-precipitation and hydrothermal methods

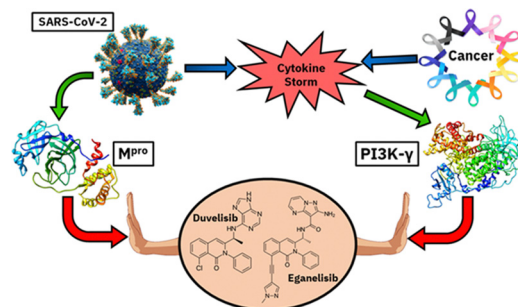
Katarzyna Szyszka* and Rafal J. Wiglusz*



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Can Duvelisib and Eganelisib work for both cancer and COVID-19? Molecular-level insights from MD simulations and enhanced samplings

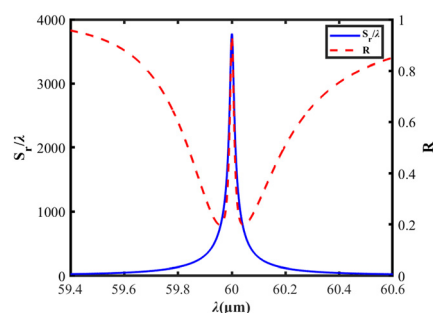
Saroj Kumar Panda, Shaswata Karmakar, Parth Sarthi Sen Gupta and Malay Kumar Rana*



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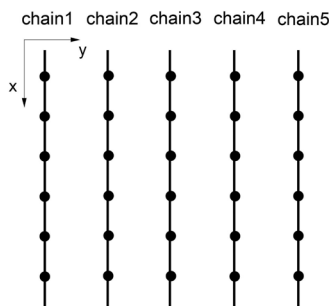
Coexistence of giant Goos–Hänchen shift and high reflectance in Dirac semimetal based multilayered structure

Dekang Yin, Wentao Liu, Mengru Zhang and Haixia Da*



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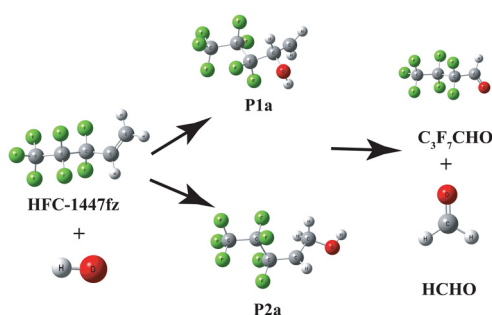
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Surface hopping simulations on charge photogeneration in conjugated polymers

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

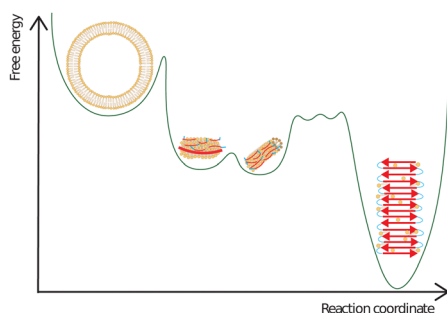
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The mechanism and kinetics of the atmospheric oxidation of $\text{CF}_3(\text{CF}_2)_2\text{CH}=\text{CH}_2$ (HFC-1447fz) by hydroxyl radicals: *ab initio* investigation

Youqing Yu,* Li Pan, Qiyao Sun and Jie Wang

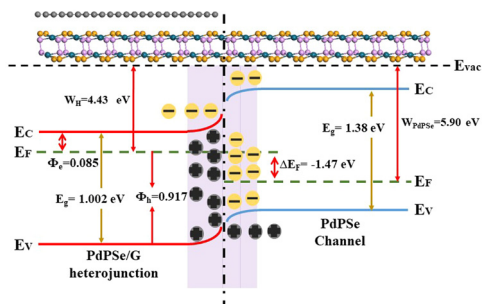
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Structural characterisation of α -synuclein–membrane interactions and the resulting aggregation using small angle scattering

Céline Galvagnion,* Abigail Barclay, Katarzyna Makasewicz, Frederik Ravnkilde Marlet, Martine Moulin, Juliette M. Devos, Sara Linse, Anne Martel, Lionel Porcar, Emma Sparr, Martin Cramer Pedersen, Felix Roosen-Runge, Lise Arleth and Alexander K. Buell*

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Contact evaluation of the penta-PdPSe/graphene vdW heterojunction: tuning the Schottky barrier and optical properties

Arzoo Hassan, Yaguang Guo, Umer Younis, Andleeb Mehmood, Xiaoqing Tian* and Qian Wang*

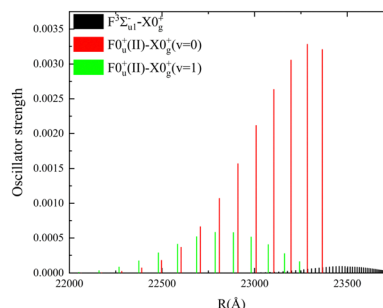


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Ab initio calculations of the spectra and lifetimes of the lead dimer

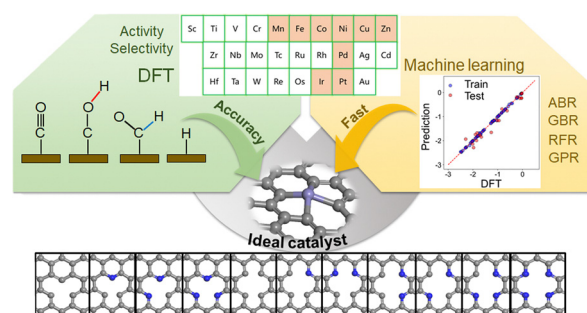
Lidan Xiao, Boris F. Minaev,* Hans Ågren and Bing Yan*



11037

Micro-kinetic modelling of the CO reduction reaction on single atom catalysts accelerated by machine learning

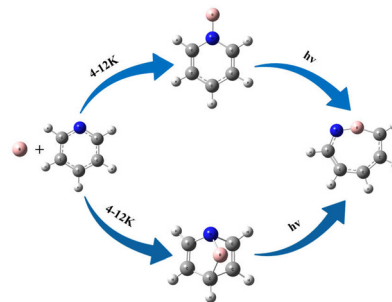
Qing-Meng Zhang, Zhao-Yu Wang, Hao Zhang,* Xiao-Hong Liu,* Wei Zhang and Liu-Bin Zhao*



11048

Synthesis and characterization of azaborepin radicals in solid neon through boron-mediated C–N bond cleavage of pyridine

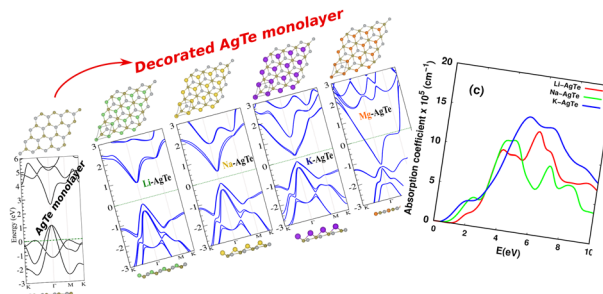
Xin Xu, Yi-Kang Zhu, Chuan-Ming Dai, Jiaping Xu and Jiwen Jian*



11056

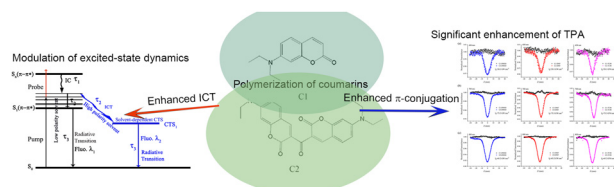
Metal to semiconductor switching in the AgTe monolayer via decoration with alkali metal and alkaline earth metal atoms: a first-principles perspective

A. Bafekry,* M. M. Fadlallah, M. Faraji, S. Hasan Khan, H. R. Jappor, Babak Shokri, M. Ghergherehchi* and Gap Soo Chang



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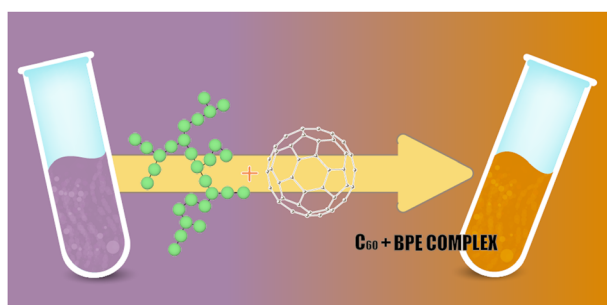
11064



Study of two-photon absorption and excited-state dynamics of coumarin derivatives: the effect of monomeric and dimeric structures

Jidong Jia,* Jie Li, Tianwei Zhang, YinLin Lu and Yinglin Song*

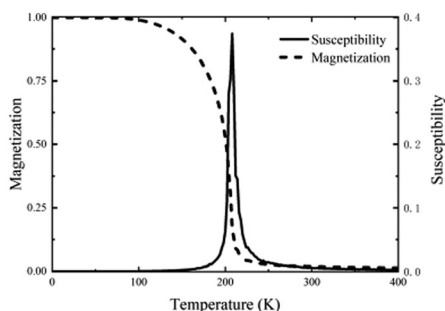
11073



Supramolecular complexation of C_{60} with branched polyethylene

Adam A. Pollit, Garima Garg, M. Nazir Tahir, Audithya Nyayachavadi, Peng Xiang, Eric Landry, Amer Ebied and Simon Rondeau-Gagné*

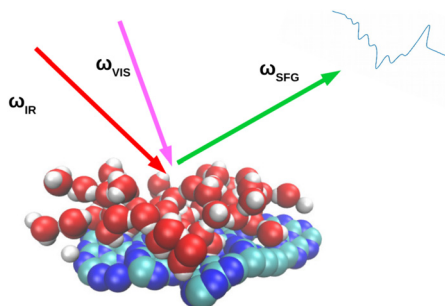
11078



Study of the magnetism of C-doped MgO based on first-principles calculations and the Ising model

Rui-Da Chen, Jia-Jun Mo and Fei Mao*

11084



Vibrational dynamics and spectroscopy of water at porous g- C_3N_4 and C_2N surfaces

Deepak Ojha, Christopher Penschke and Peter Saalfrank*

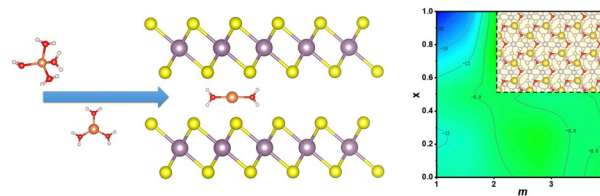


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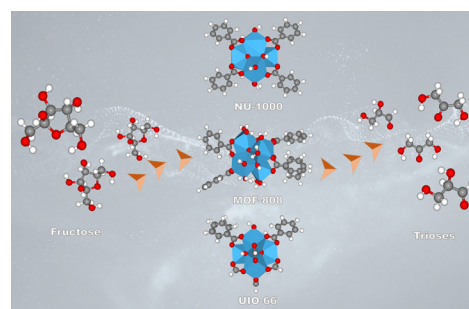
11094

Morphology and selectivity of hydrated alkali metal ions as depth of discharge in the 1T-MoS₂ electrode with aqueous electrolytes

Shenrui Liao, Wenhui Zhao* and Xiao Gu*



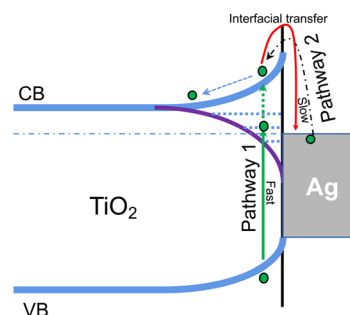
11105

Theoretical study of fructose adsorption and conversion to trioses on metal–organic frameworksJarinya Sittiwong, Thana Maihom,*
Chomphunuch Wansa, Michael Probst and
Jumras Limtrakul

11113

Kinetic pathways of sub-bandgap induced electron transfer in Ag/TiO₂ and the effect on isopropanol dehydrogenation under gaseous conditions

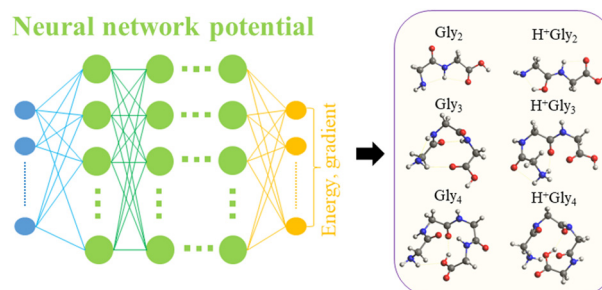
Liping Wen and Baoshun Liu*



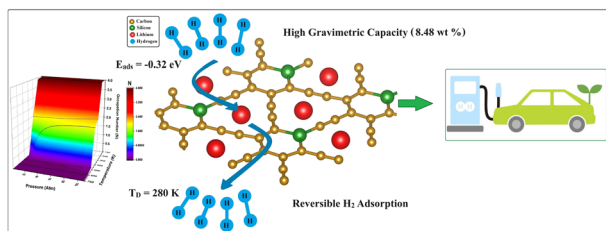
11126

Searching low-energy conformers of neutral and protonated di-, tri-, and tetra-glycine using first-principles accuracy assisted by the use of neural network potentials

Hieu Cao Dong, Po-Jen Hsu and Jer-Lai Kuo*



11140



Lithium-grafted Si-doped γ -graphyne as a reversible hydrogen storage host material

Nidhi Duhan and T. J. Dhilip Kumar*

