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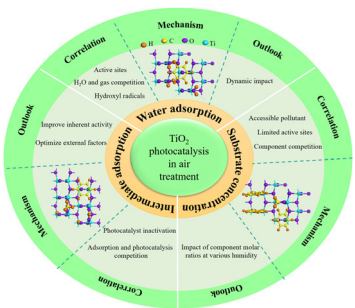
Zhifeng Lin, Xueding Jiang,* Weicheng Xu, Fuhua Li, Xin Chen, Hailong Wang, Si Liu* and Xihong Lu*



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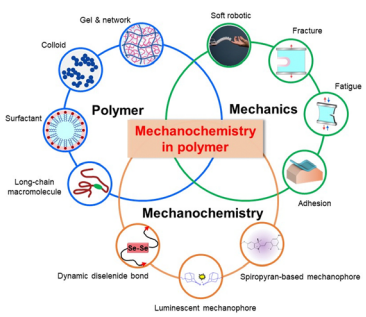
Qifeng Mu* and Jian Hu*



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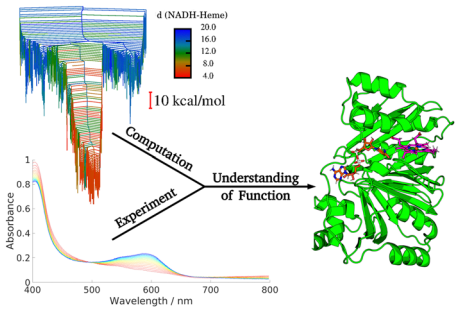
Alasdair D. Keith,* Elizabeth B. Sawyer, Desmond C. Y. Choy, Yuhang Xie, George S. Biggs, Oskar James Klein, Paul D. Brear, David J. Wales* and Paul D. Barker*



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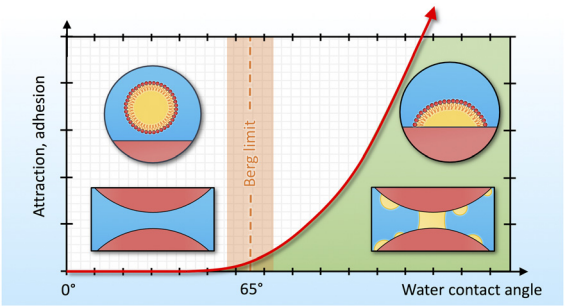
Matej Kanduč,* Emanuel Schneck and Roland R. Netz



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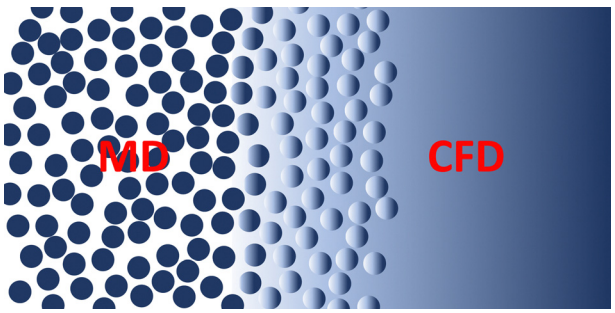
Multiscale simulation of fluids: coupling molecular and continuum

Edward R. Smith* and Panagiotis E. Theodorakis*



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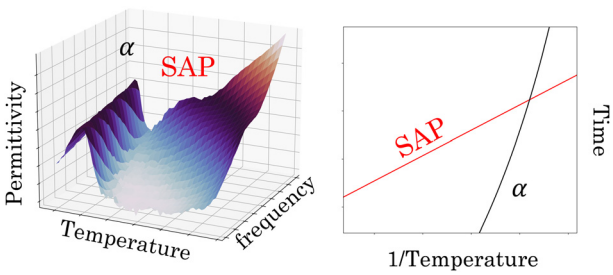
The slow Arrhenius process in small organic molecules

Federico Caporaletti* and Simone Napolitano*



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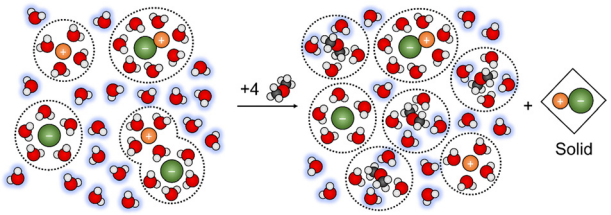

Modeling Henry's law and phase separations of water–NaCl–organic mixtures with solvation and ion-pairing

Aaron D. Wilson,* Zi Hao Foo, Ashini S. Jayasinghe, Caleb Stetson, Hyeonseok Lee, Harry W. Rollins, Akshay Deshmukh and John H. Lienhard

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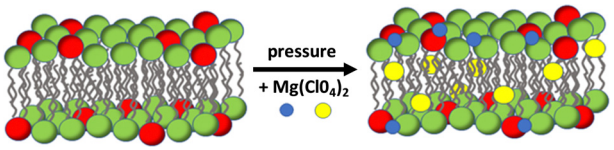

Bacterial model membranes under the harsh subsurface conditions of Mars

Attila Tortorella, Rosario Oliva, Concetta Giancola,* Luigi Petraccone* and Roland Winter*

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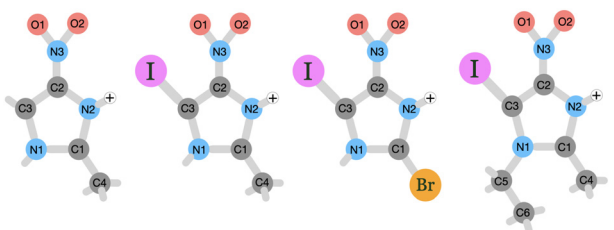

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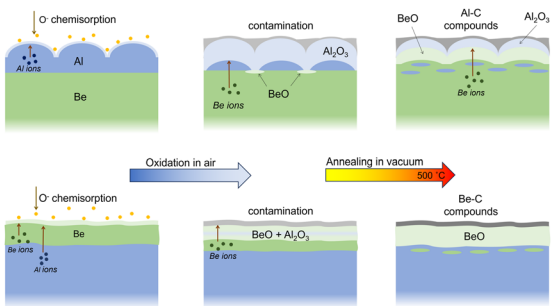

Effect of low-temperature oxidation and heat treatment under vacuum on the Al–Be interdiffusion process

Aidar U. Gaisin and Elena O. Filatova*

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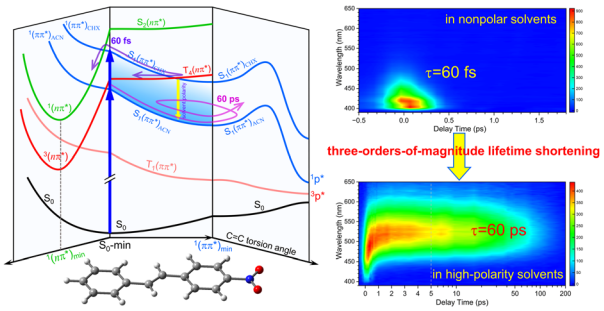
Peng-Yun Wang, Yu-Cheng Hsu, Pin-Hsun Chen, Guan-Yu Chen, Yi-Kai Liao and Po-Yuan Cheng*



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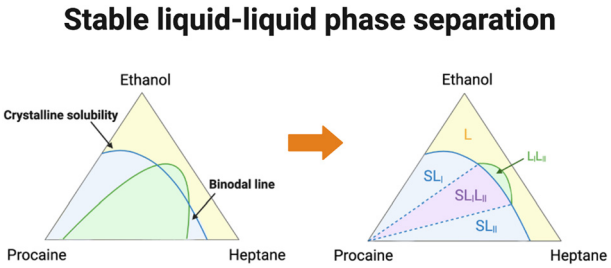
Complex oiling-out behavior of procaine with stable and metastable liquid phases

Da Hye Yang, Francesco Ricci, Fredrik L. Nordstrom and Na Li*



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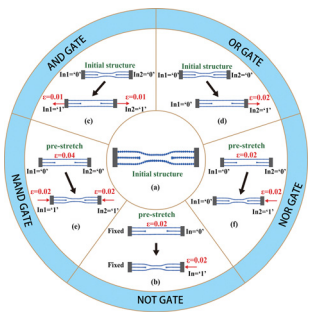
Flexible nanomechanical bit based on few-layer graphene

Bin Zhang, Yixuan Xue,* Harold S. Park* and Jin-Wu Jiang*



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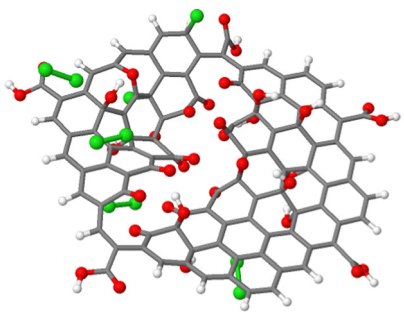
ClO-driven degradation of graphene oxide: new insights from DFT calculations

S. L. Romo-Ávila, D. Márquez-Ruíz and R. A. Guirado-López*



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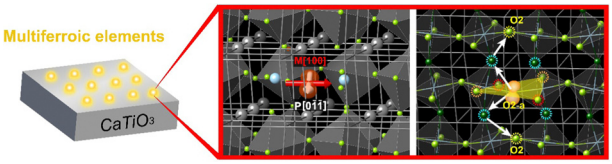

Emergent ultrasmall multiferroics in paraelectric perovskite oxide by hole polarons

Tao Xu,* Masataka Mori, Hiroyuki Hirakata, Takayuki Kitamura and Takahiro Shimada*

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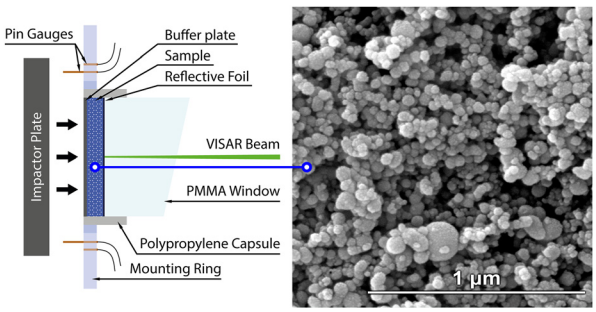

Effect of porosity on rapid dynamic compaction of nickel nanopowder

Timofei Rostilov,* Vadim Ziborov, Alexander Dolgoborodov and Mikhail Kuskov

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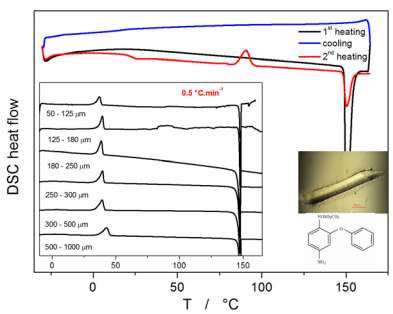

Thermal stability of amorphous nimesulide: from glass formation to crystal growth and thermal degradation

Roman Svoboda,* Jana Macháčková, Marie Nevyhoštěná and Alena Komersová

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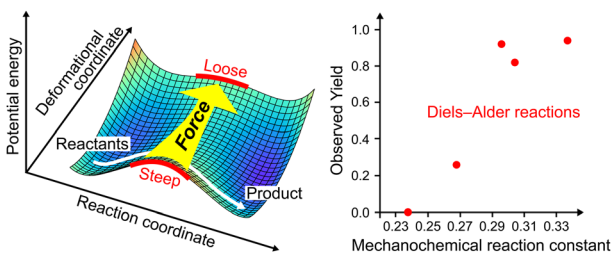

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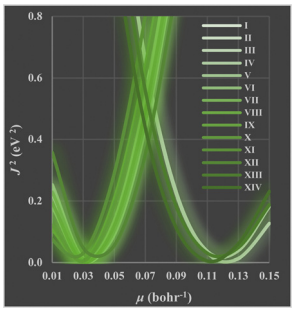
Mahdi Soltani Nejad and Mojtaba Alipour*



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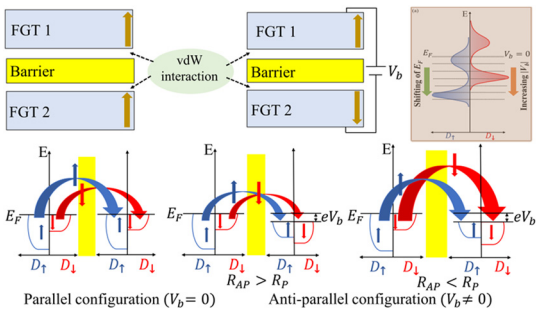
Tunable long-range spin transport in a van der Waals $Fe_3GeTe_2/WSe_2/Fe_3GeTe_2$ spin valve

Anil Kumar Singh, Weibo Gao and Pritam Deb*



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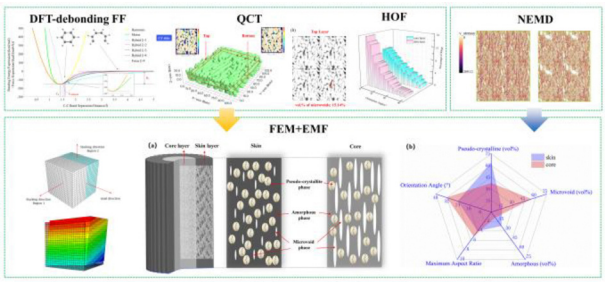
Atomistically informed hierarchical modeling for revisiting the constituent structures from heredity and nano–micro mechanics of sheath-core carbon fiber

Pengcheng Shi, Youqiang Yao, Yingdan Zhu,* Xiaochen Yu, Dong Liu, Chun Yan and Gang Chen



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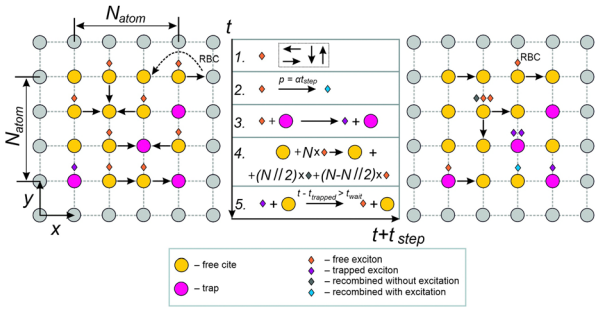
Negative diffusion of excitons in quasi-two-dimensional systems

Aleksandr A. Kurilovich, Vladimir N. Mantsevich, Aleksei V. Chechkin and Vladimir V. Palyulin*



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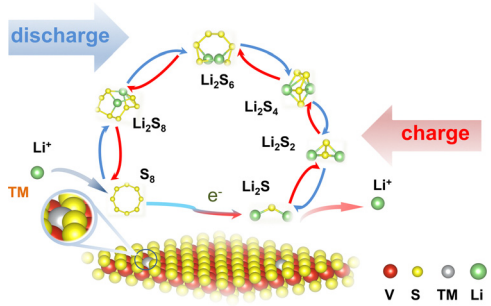

Theoretical study of highly efficient VS_2-based single-atom catalysts for lithium–sulfur batteries

Yao Liu, Yang Li, Jinhui Zhang, Jing Xu* and Dashuai Wang*

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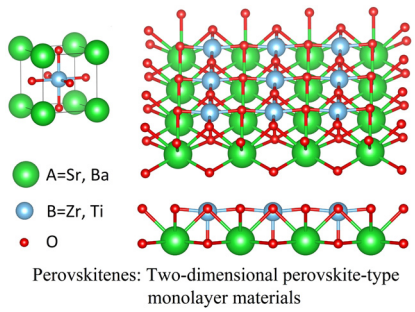

Perovskitenes: Two-dimensional perovskite-type monolayer materials

Perovskenes: two-dimensional perovskite-type monolayer materials predicted by first-principles calculations

Mosayeb Naseri,* Shirin Amirian, Mehrdad Faraji, Mohammad Abdur Rashid, Maicon Pierre Lourenço, Venkataraman Thangadurai and D. R. Salahub*

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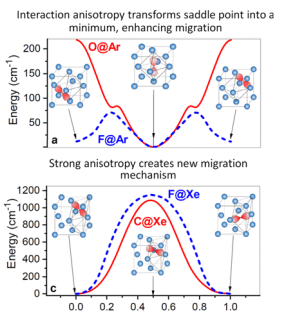

Trapping and thermal migration of the first- and second-row atoms in Ar, Kr and Xe crystals

Iosif V. Leibin,* Dmitry S. Bezrukov and Alexei A. Buchachenko

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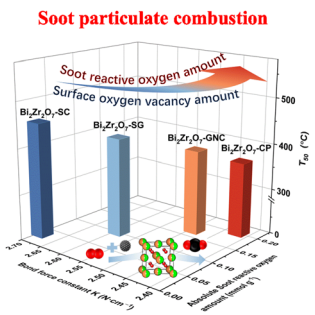

The controlled engineering of surface oxygen defects on $Bi_2Zr_2O_7$ compounds for catalytic soot combustion by adjusting the preparation methods

Shijing Zhang, Xiaohui Feng, Zekai Xu, Yuting Li, Ping Wang, Jiating Shen, Junwei Xu, Xianglan Xu, Xiuzhong Fang and Xiang Wang*

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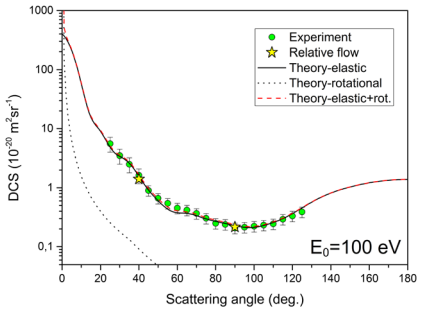
Investigating theoretical and experimental cross sections for elastic electron scattering from isoflurane

Jelena Vukalović,* Bratislav P. Marinković, Jaime Rosado, Francisco Blanco, Gustavo García and Jelena B. Maljković



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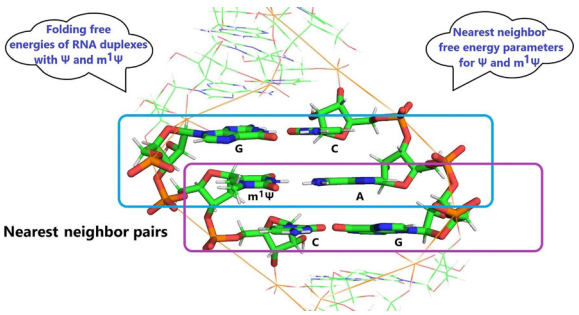
Predicting nearest neighbor free energies of modified RNA with LIE: results for pseudouridine and *N*1-methylpseudouridine within RNA duplexes

Nivedita Dutta, Joanna Sarzynska, Indrajit Deb and Ansuman Lahiri*



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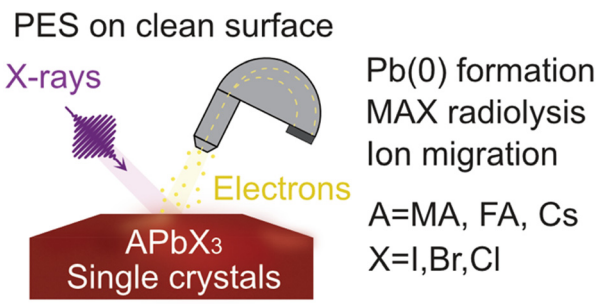
Composition dependence of X-ray stability and degradation mechanisms at lead halide perovskite single crystal surfaces

Alberto García-Fernández, Birgit Kammlander, Stefania Riva, Håkan Rensmo and Ute B. Cappel*



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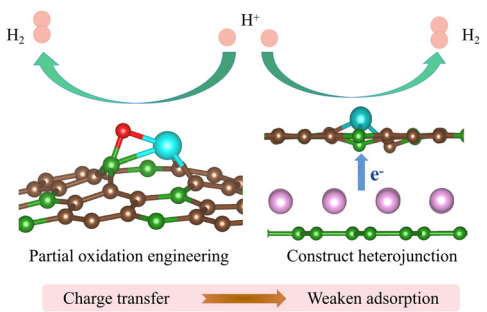
HER catalytic activity and regulation of a transition metal atom-anchored BC_3 monolayer: a first-principles study

Liying Pan, Xuxin Kang, Shan Gao* and Xiangmei Duan*



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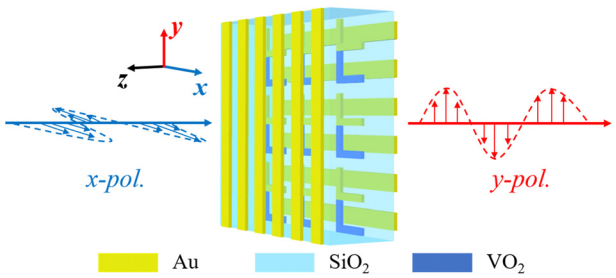

Switchable asymmetric transmission with broadband polarization conversion in vanadium dioxide-assisted terahertz metamaterials

Zhichao Liu, Tianle Zhou, Gui Jin, Jiangbin Su and Bin Tang*

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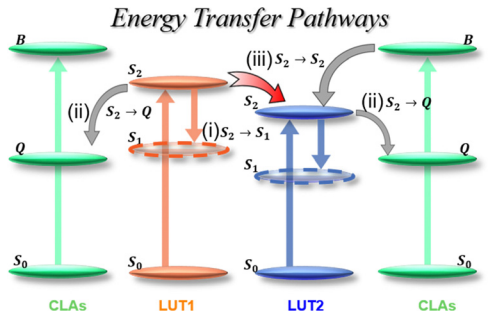

Energy transfer from two luteins to chlorophylls in light-harvesting complex II study by using exciton models with phase correction

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

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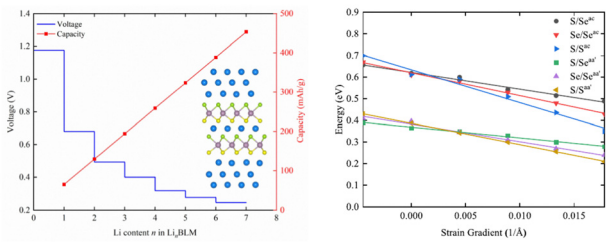

Tunable Li-ion diffusion properties in MoSSe bilayer anodes by strain gradient

Li Zhong, Xiaobao Li,* Yuxue Pu, Meiqin Wang, Chunxiao Zhan and Xinle Xiao*

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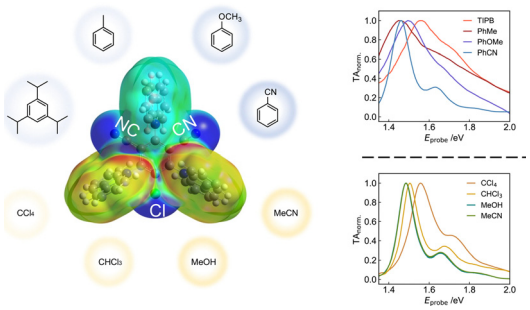

Solvent effects on the intramolecular charge transfer excited state of 3CzClIPN: a broadband transient absorption study

Ruofei Zheng, Meixin Cheng, Ruishu Ma, Derek Schipper, Kostyantyn Pichugin and Germán Sciaini*

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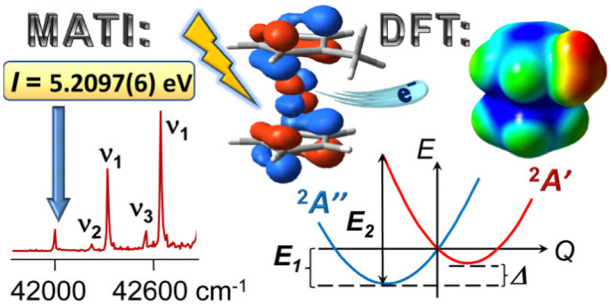
Effect of a single methyl substituent on the electronic structure of cobaltocene studied by computationally assisted MATI spectroscopy

Sergey Yu. Ketkov,* Sheng-Yuan Tzeng, Elena A. Rychagova, Anton N. Lukoyanov and Wen-Bih Tzeng*



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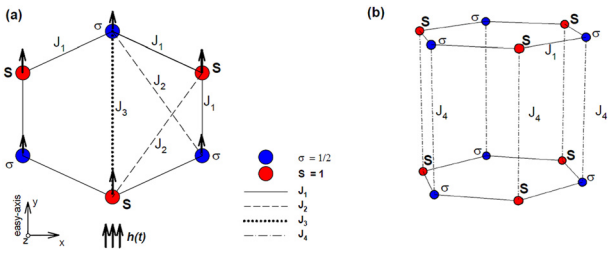
Non-equilibrium magnetic properties of a mixed spin (1/2, 1) Ising graphene nanoisland

Bayram Deviren,* Seyma Akkaya Deviren and Tevfik Fikret Yagmuroglu



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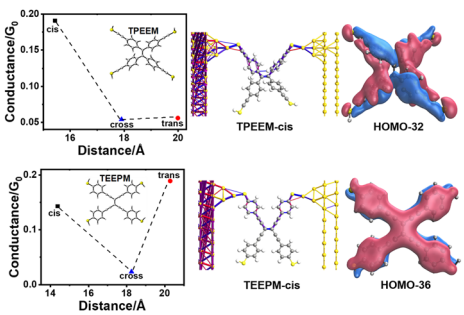
The effect of weak π–π interactions on single-molecule electron transport properties of the tetraphenylethene molecule and its derivatives: a first-principles study

Zhiye Wang, Yunchuan Li* and Mingjun Sun*



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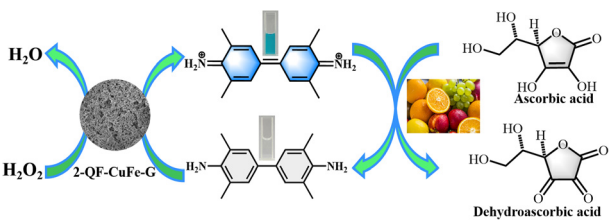
Peroxidase activity of a Cu–Fe bimetallic hydrogel and applications for colorimetric detection of ascorbic acid

Xiao-Juan Wang, Yan Long, Chuan-Wan Wei,* Shu-Qin Gao and Ying-Wu Lin*



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A novel 2D intrinsic metal-free ferromagnetic semiconductor Si_3C_8 monolayer

Yangtong Luo, Chen Li, Chengyong Zhong* and Shuo Li*

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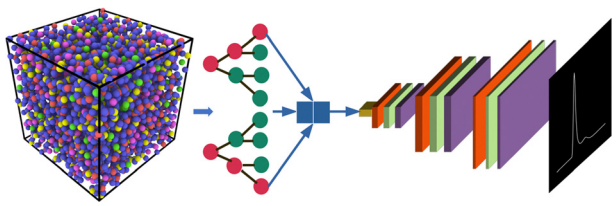

Predicting the pair correlation functions of silicate and borosilicate glasses using machine learning

Kumar Ayush, Pooja Sahu, Sk. Musharaf Ali* and Tarak K. Patra*

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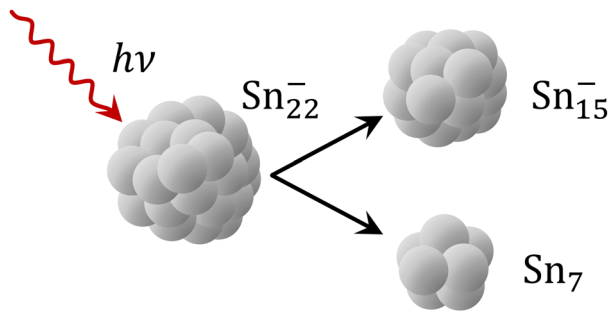

Delayed photodissociation of the tin cluster Sn_{22}^-

Alexander Jankowski,* Paul Fischer, Klavs Hansen and Lutz Schweikhard

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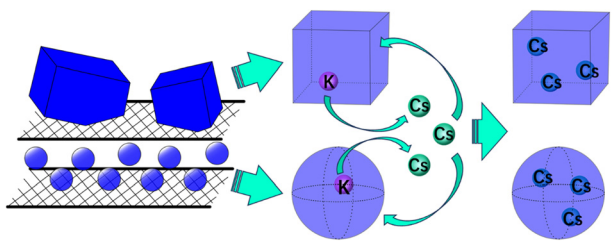

A Prussian blue analog-based copper–aluminum layered double hydroxide for cesium removal from water: fabrication, density functional theory-based molecular modeling, and the adsorption mechanism

Xindai Li, Kexin Shao, Guangming Xu, Meng Xia, Xinyao Liu, Zhaorong Shang, Fuqiang Fan* and Junfeng Dou*

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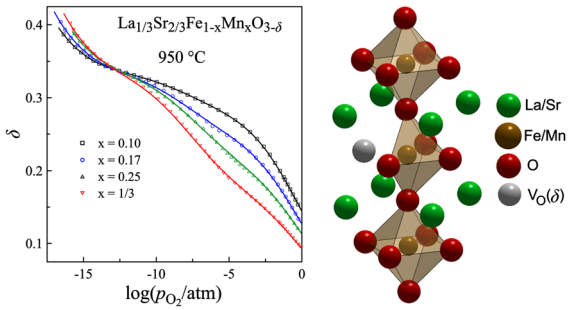
The effect of temperature and oxygen partial pressure on the concentration of iron and manganese ions in $La_{1/3}Sr_{2/3}Fe_{1-x}Mn_xO_{3-\delta}$

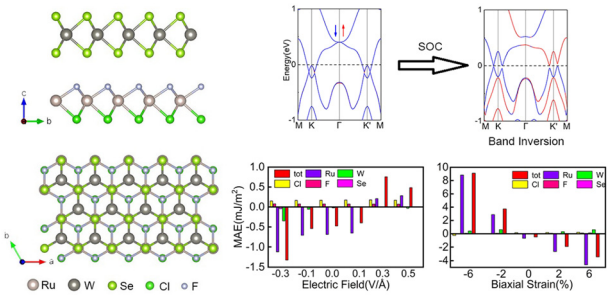
Sergey S. Nikitin,* Alexander D. Koryakov, Elizaveta A. Antipinskaya, Alexey A. Markov and Mikhail V. Patrakeev



1135

Band inversion and switchable magnetic properties of two-dimensional RuClF/WSe_2 van der Waals heterostructures

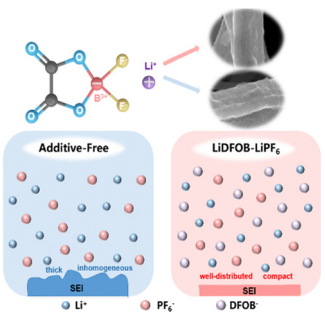
Ziyu Liu, Baozeng Zhou, Xiaocha Wang* and Wenbo Mi*



1148

Insights into the multi-functional lithium difluoro(oxalate)borate additive in boosting the Li-ion reaction kinetics for Li_3VO_4 anodes

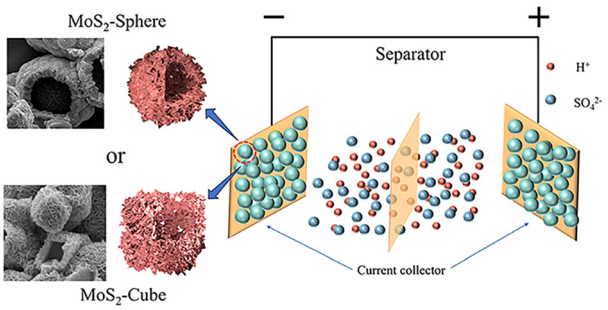
Miaomiao Zhang, Cunyuan Pei,* Qiqi Xiang, Lintao Liu, Zhongxu Dai,* Huijuan Ma and Shibing Ni*



1156

Designed fabrication of MoS_2 hollow structures with different geometries and the comparative investigation toward capacitive properties

Yuandong Xu,* Haoyang Feng, Chaoyang Dong, Yuqing Yang, Meng Zhou, Yajun Wei,* Hui Guo, Yaqing Wei, Jishan Su, Yingying Ben and Xia Zhang*



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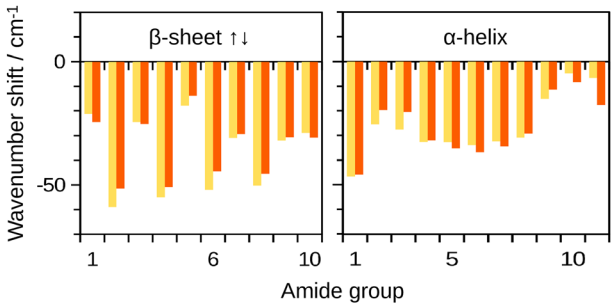
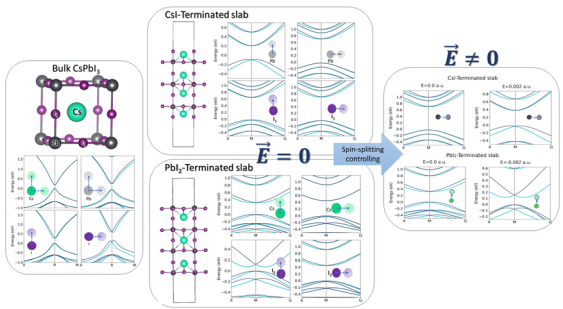


Refining protein amide I spectrum simulations with simple yet effective electrostatic models for local wavenumbers and dipole derivative magnitudes

Cesare M. Baronio and Andreas Barth*

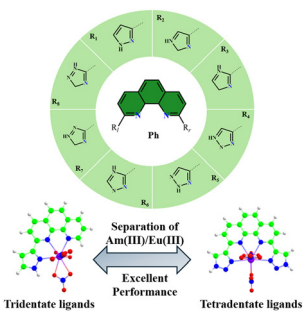
1182



Unravelling the band splitting origin in bulk and 2D distorted α-$CsPbI_3$ perovskite

Safieh Nazari,* Fatemeh Mohammad Dezashibi and Nadia Babaei Bidmeshki

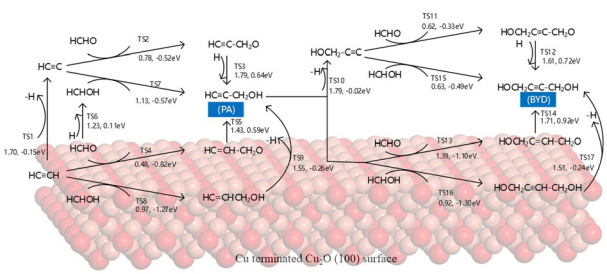
1190



Theoretical investigation on the ligands constructed from phenanthroline and five-membered N-heterocyclic rings for bonding and separation properties of Am(III) and Eu(III)

Shouqiang Wu and An Yong Li*

1205



Reaction mechanism of the ethynylation of formaldehyde on copper terminated Cu_2O(100) surfaces: a DFT study

Minhua Zhang, Qin Yang, Ruishen Li and He Dong*

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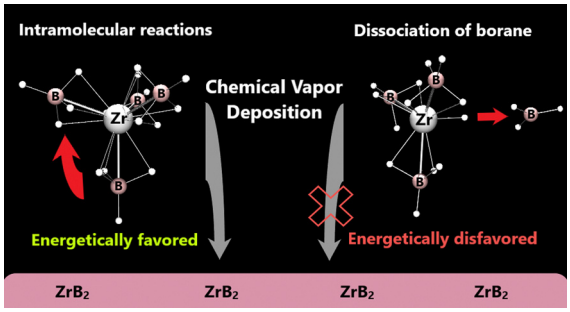
1217

Early events in the mechanism of single-source chemical vapor deposition of zirconium and hafnium diboride: a computational investigation

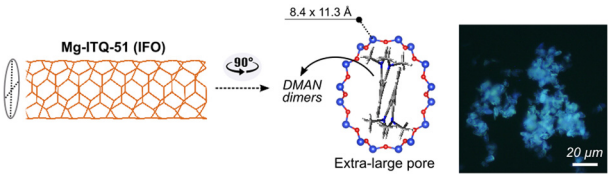
Sergei Prokvolit, Erqian Mao and Thomas G. Gray*



1225

Exploiting the photophysical features of DMAN template in ITQ-51 zeotype in the search for FRET energy transfer

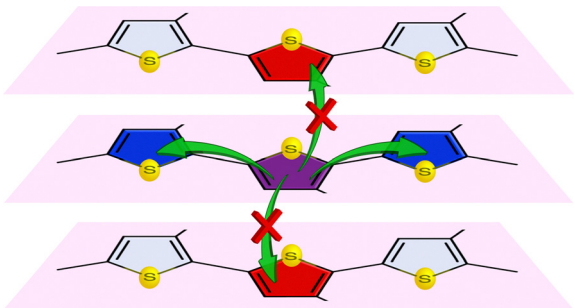
Ainhoa Oliden-Sánchez, Rebeca Sola-Llano, Joaquín Pérez-Pariente, Luis Gómez-Hortigüela* and Virginia Martínez-Martínez*



1234

X-ray induced ultrafast charge transfer in thiophene-based conjugated polymers controlled by core-hole clock spectroscopy

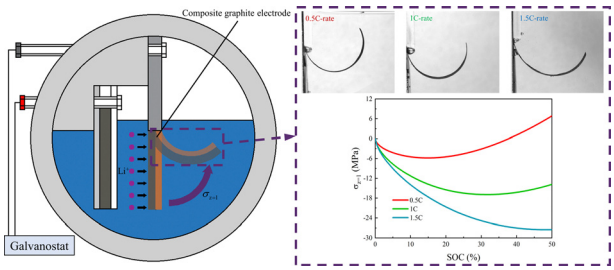
Nicolas Velasquez, Fernanda B. Nunes, Oksana Travnikova, Iyas Ismail, Renaud Guillemin, Jessica B. Martins, Denis Céolin, Loïc Journel, Laure Fillaud, Dimitris Koulentianos, Chinnathambi Kamal, Ralph Püttner, Maria Novella Piancastelli, Marc Simon, Michael Odelius, Marcella Iannuzzi and Tatiana Marchenko*



1245

Effect of the charge rate on the mechanical response of composite graphite electrodes: *in situ* experiment and mathematical analysis

Hainan Jiang, Yaolong He, Xiaolin Li, Zhiyao Jin, Huijie Yu* and Dawei Li*



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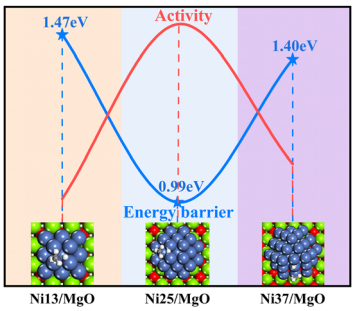
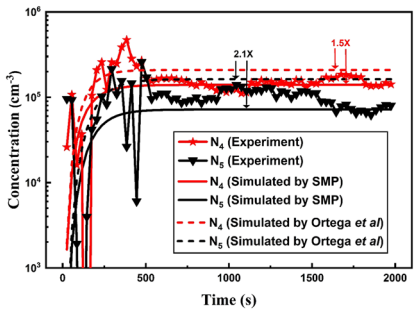


Unraveling the effect of particle size of active metals in Ni/MgO on methane activation and carbon growth mechanism

Shengzhuo Chen, Juntian Niu,* Xianrong Zheng, Haiyu Liu, Yan Jin and Jingyu Ran

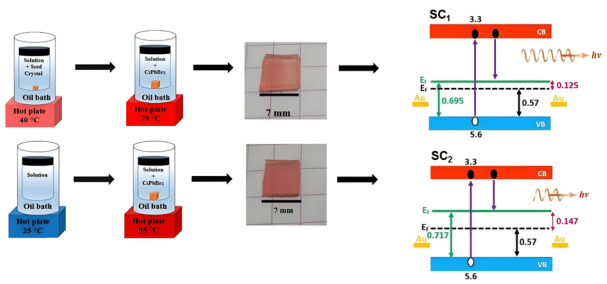
1267



Growth mechanism prediction for nanoparticles *via* structure matching polymerization

Yi-Rong Liu* and Yan Jiang

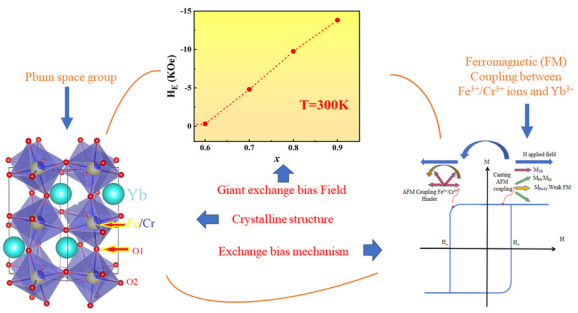
1274



Growth methods' effect on the physical characteristics of $CsPbBr_3$ single crystal

Mohamed Ben Bechir* and Faisal Alresheedi

1284



Giant exchange bias field above room temperature in perovskite $YbCr_{1-x}Fe_xO_3$ (x = 0.6–0.9)

Kang Zhao, Dao Wang, Lei Wang* and Sajjad Ur Rehman*

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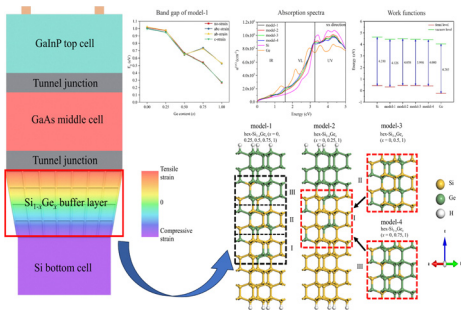
1293

A study on the $Si_{1-x}Ge_x$ gradual buffer layer of III–V/Si multi-junction solar cells based on first-principles calculations

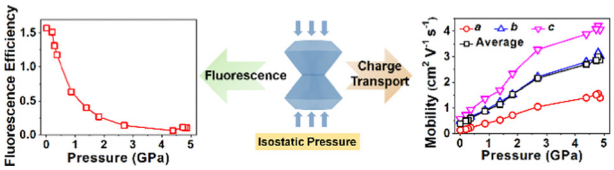
Qian Wang, Yu Zhuang,* Abuduwayiti Aierken,* Qiaogang Song, Qin Zhang, Youbo Dou, Qiuli Zhang and Shuyi Zhang



1303

Pressure effects on both fluorescent emission and charge transport properties of organic semiconductors: a computational study

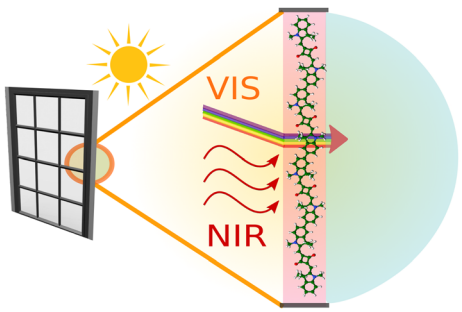
Yi Zeng, Wen Shi, Qian Peng, Yingli Niu, Zhiying Ma and Xiaoyan Zheng*



1314

Design of J-aggregates-like oligomers built from squaraine dyes exhibiting transparency in the visible regime and high fluorescence quantum yield in the NIR region

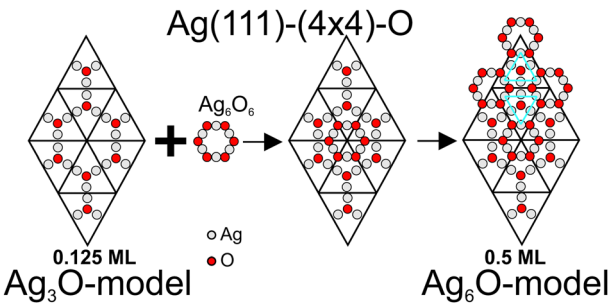
Margarita Bužančić Milosavljević and Vlasta Bonačić-Koutecký*



1322

New insights into the structure of the Ag(111)-*p*(4 × 4)-O phase: high-resolution STM and DFT study

B. V. Andryushechkin,* T. V. Pavlova and V. M. Shevlyuga



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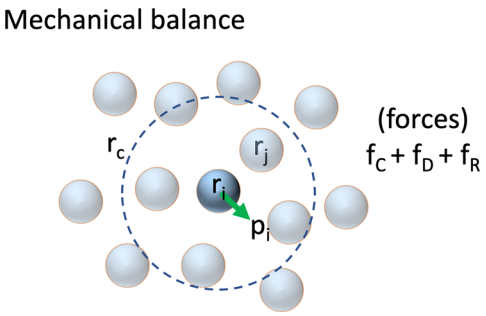
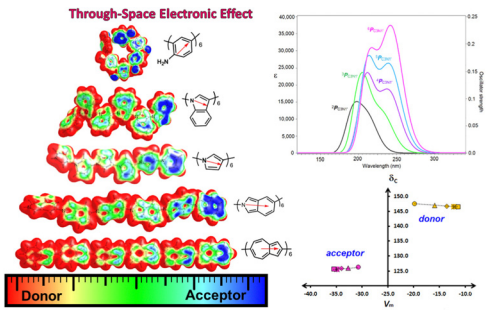
1328



Green–Kubo expressions for transport coefficients from dissipative particle dynamics simulations revisited

D. C. Malaspina, M. Lísal, J. P. Larentzos, J. K. Brennan, A. D. Mackie and J. Bonet Avalos*

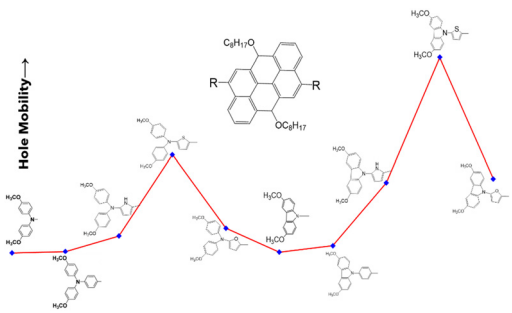
1340



Utilization of the through-space effect to design donor–acceptor systems of pyrrole, indole, isoindole, azulene and aniline

Puthannur K. Anjalikrishna and Cherumuttathu H. Suresh*

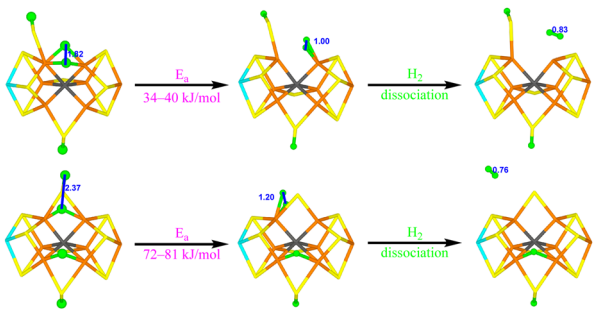
1352



Effect of substituting donors on the hole mobility of hole transporting materials in perovskite solar cells: a DFT study

Md Al Mamunur Rashid, Sein Min, Sung Keon Namgoong and Keunhong Jeong*

1364



H_2 formation from the E_2–E_4 states of nitrogenase

Hao Jiang and Ulf Ryde*

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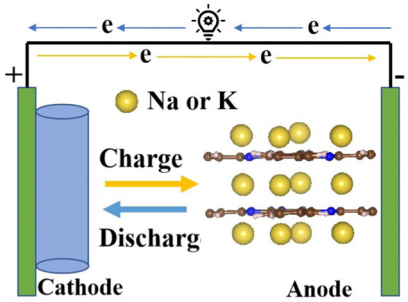
1376

First principles study of a triazine-based covalent organic framework as a high-capacity anode material for Na/K-ion batteries

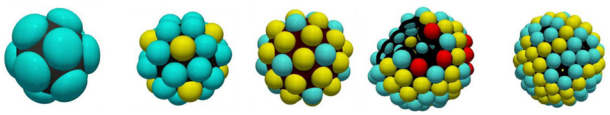
Sitong Liu, Bo Liu,* Meidong Yu, Hanyu Gao, Haipeng Guo, Daguo Jiang, Shenbo Yang, Yufeng Wen* and Yabei Wu



1385

Breaking the size constraint for nano cages using annular patchy particles

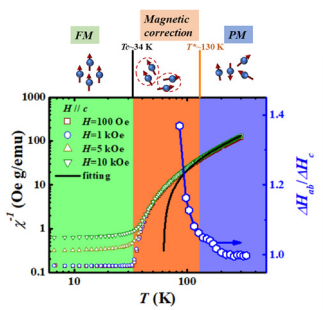
Vikki Anand Varma, Simmie Jaglan, Mohd Yasir Khan and Sujin B. Babu*



1396

Observation of the possible magnetic correction above the Curie temperature in $Cr_2Si_2Te_6$ single crystals

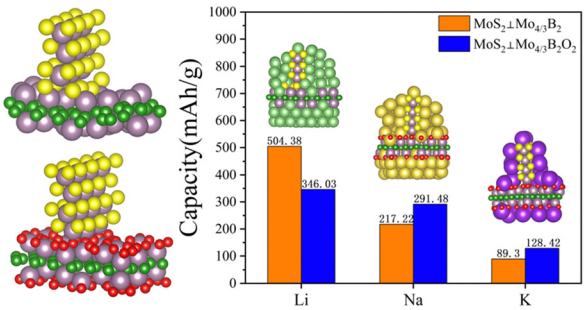
Yan Sun,* Zhongzhu Jiang, Yang Li, Lanxin Liu, Hui Liang, Yiyan Wang, Dandan Wu, Na Li, Ying Zhou, Qiuju Li, Xiaoyu Yue, Wei Tong, Xuan Luo, Jianghe Lan* and Xuefeng Sun*



1406

Improved ion adsorption capacities and diffusion dynamics in surface anchored $MoS_2 \perp Mo_{4/3}B_2$ and $MoS_2 \perp Mo_{4/3}B_2O_2$ heterostructures as anodes for alkaline metal-ion batteries

Zifeng Song, Haoliang Liu, Baiyi Chen, Qin Jiang, Fengxiang Sui, Kai Wu, Yonghong Cheng and Bing Xiao*



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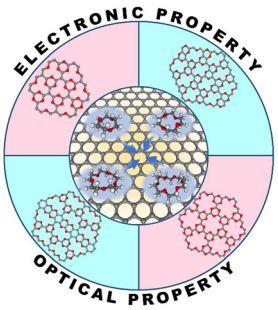
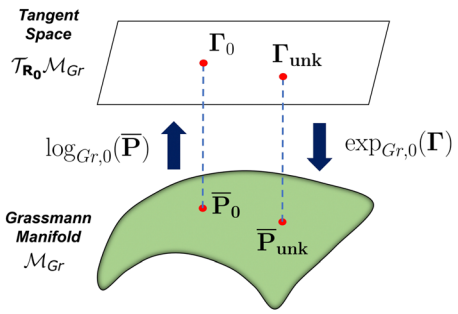


Dense arrangement of crown ethers in graphene: novel graphitic carbon oxides with enhanced optoelectronic properties

Hongyan Li, Jiang Xiang, Liang Chen, Jing Xu* and Wei Liu*

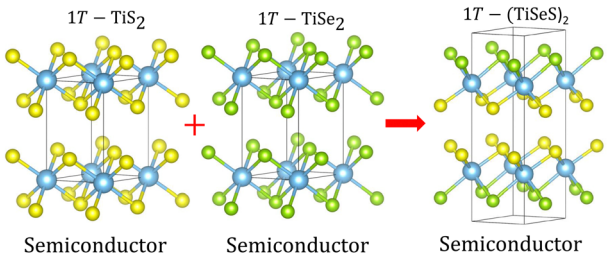
1436



Mapping spin contamination-free potential energy surfaces using restricted open-shell methods with Grassmannians

Jake A. Tan* and Ka Un Lao*

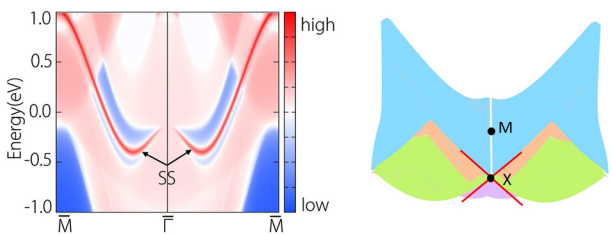
1443



Janus layers and electronic structure of 1T-$(TiSeS)_2$

Yue Lou* and Ping Lou*

1454



Coexistence of topological node surface and Dirac fermions in phonon-mediated superconductor YB_2C_2

Siqi Wang, Mingmin Zhong,* Haibo Liu and Meng Ju

CORRECTION

1462

Correction: Extracting accurate information from triplet–triplet annihilation upconversion data with a mass-conserving kinetic model

Abhishek Kalpattu, Tristan Dilbeck, Kenneth Hanson and John T. Fourkas*