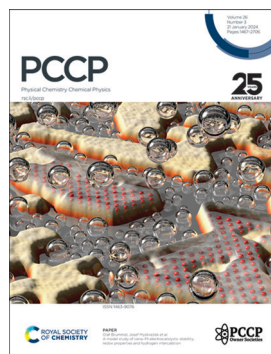


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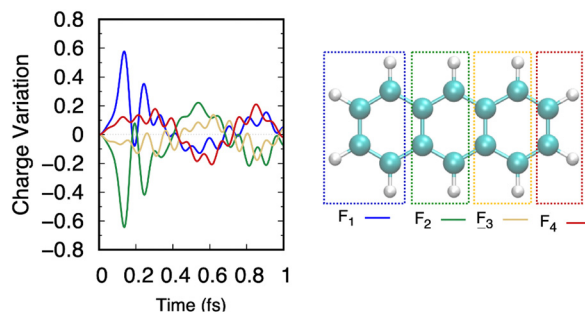
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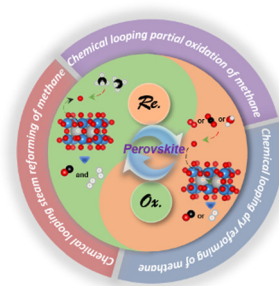
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Yuelun Li, Mingyi Chen, Lei Jiang, Dong Tian* and Kongzhai Li*



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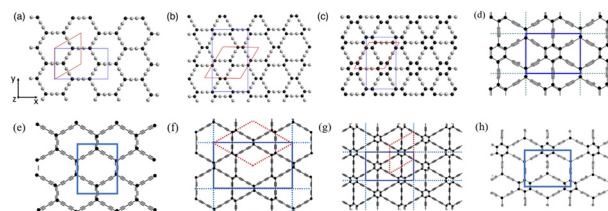
Fundamental questions
Elemental answers

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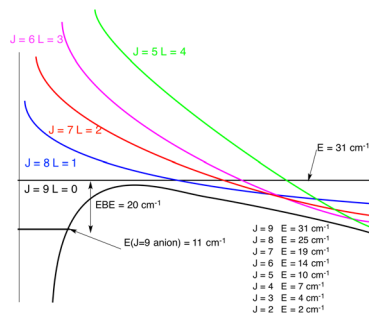


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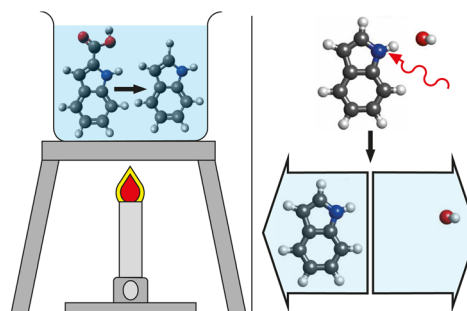
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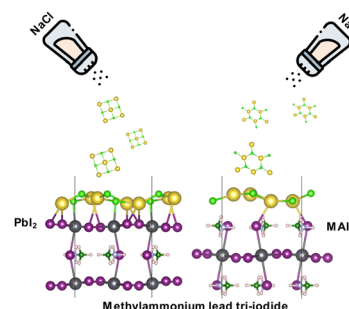
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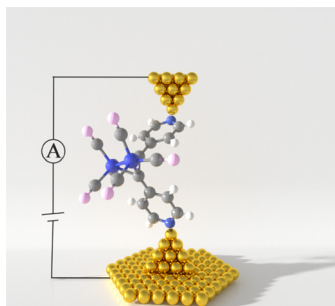


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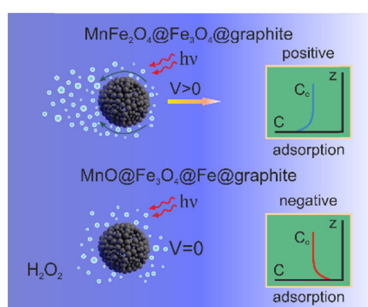
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Chaoqi Ma, Yunpeng Li, Ajun Tang, Rui Wang, Yingjie Li, Zhi Li, Jiawei Yang and Hongxiang Li*

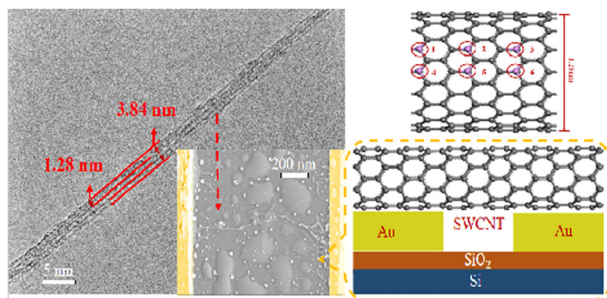
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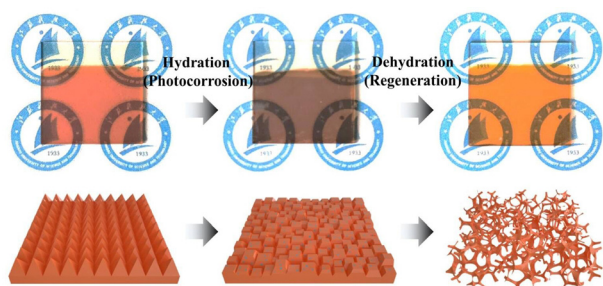
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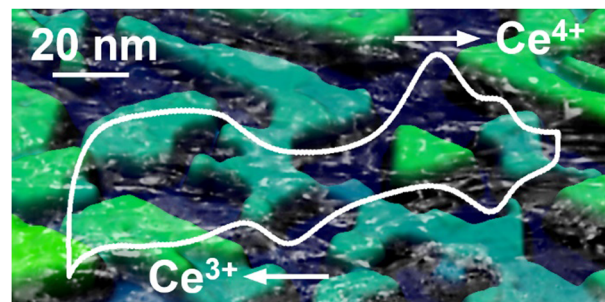


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A model study of ceria–Pt electrocatalysts: stability, redox properties and hydrogen intercalation

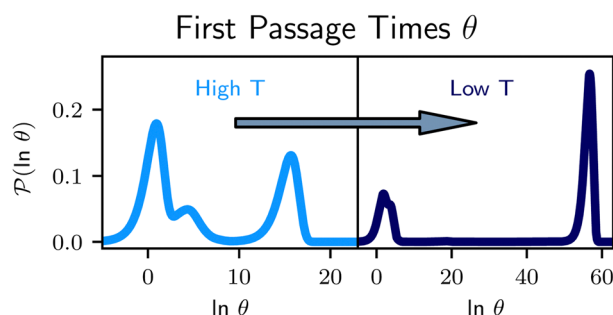
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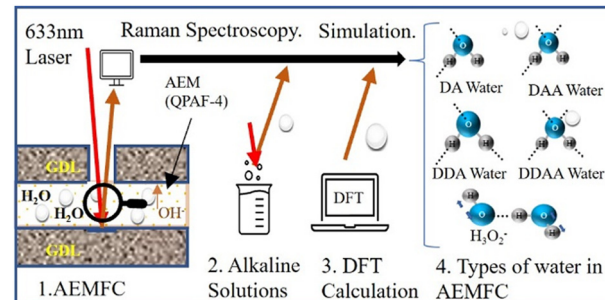
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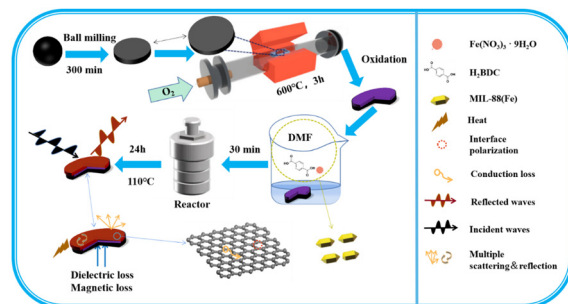
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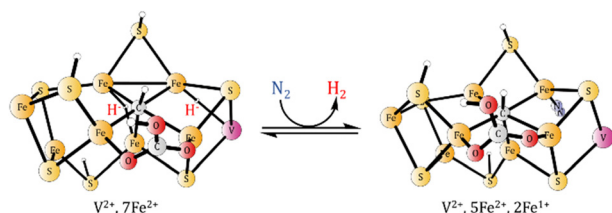
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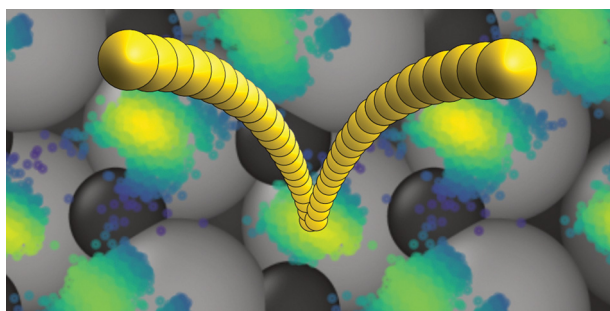
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The energetics of N_2 reduction by vanadium containing nitrogenase

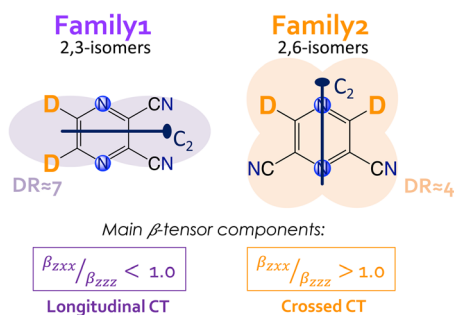
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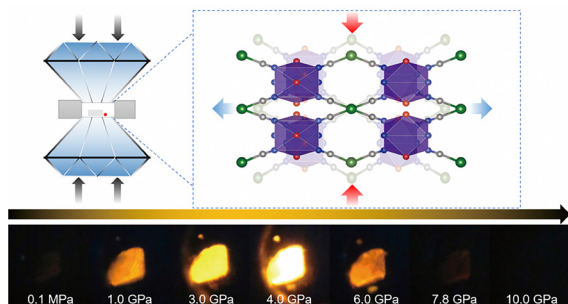
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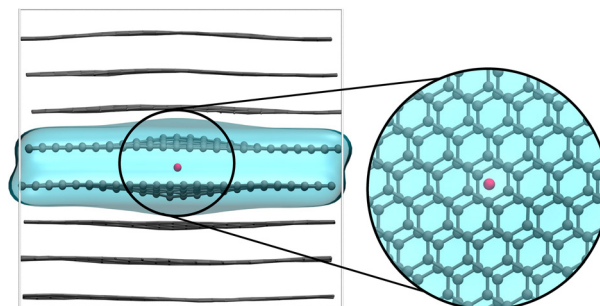


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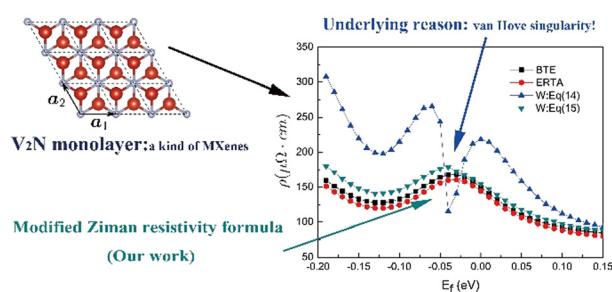
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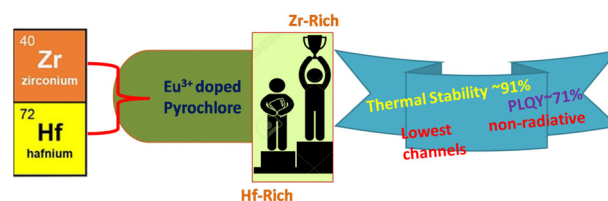
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Composition-dependent photoluminescence in nanocrystalline $La_2Hf_{2-x}Zr_xO_7:Eu$ phosphor: role of chemical twin Zr/Hf environments around a luminescent center

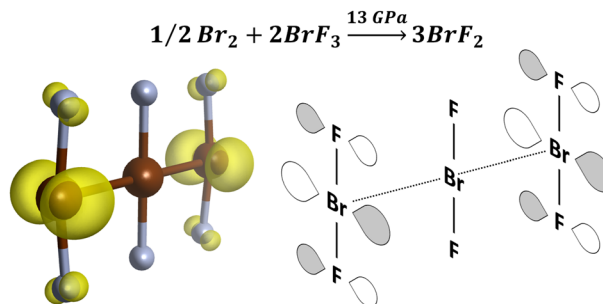
Santosh K. Gupta,* Sandeep Nigam and Yuanbing Mao



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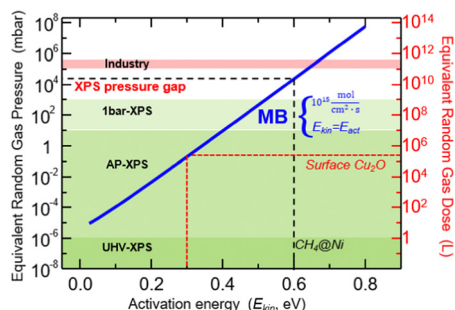
High-pressure stabilization of open-shell bromine fluorides

Madhavi H. Dalsaniya,* Deepak Upadhyay, Krzysztof Jan Kurzydowski and Dominik Kurzydowski*



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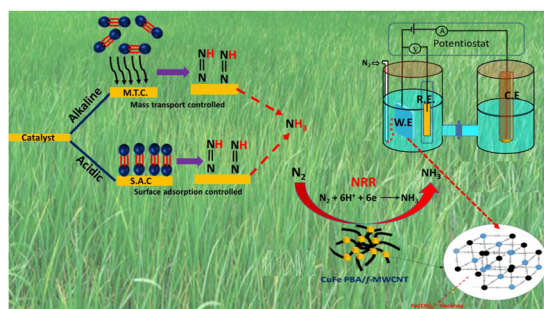
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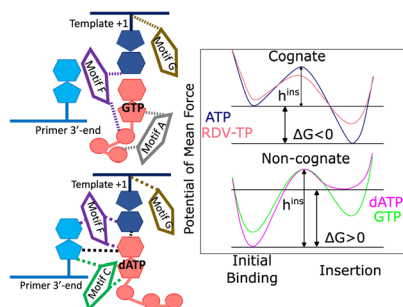
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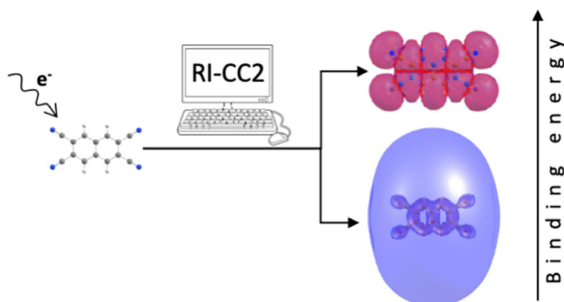
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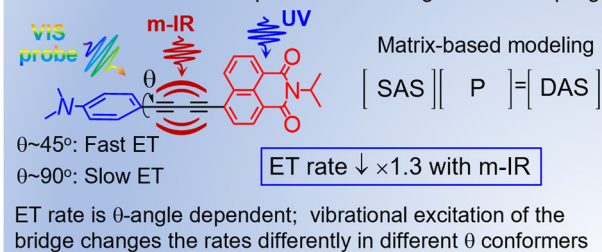
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Electron transfer rate modulation with mid-IR in butadiyne-bridged donor–bridge–acceptor compounds

Kasun C. Mendis, Xiao Li, Jesús Valdiviezo, Susannah D. Banziger, Peng Zhang, Tong Ren, David N. Beratan and Igor V. Rubtsov*

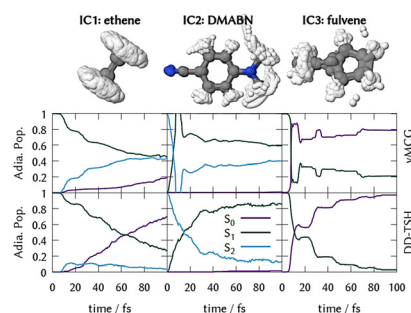
ET rate modulation in the presence of strong vibronic coupling



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Benchmarking non-adiabatic quantum dynamics using the molecular Tully models

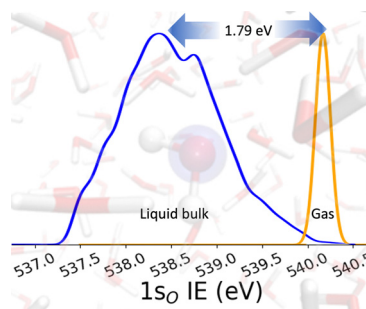
Sandra Gómez, Eryn Spinlove and Graham Worth*



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Core-ionization spectrum of liquid water

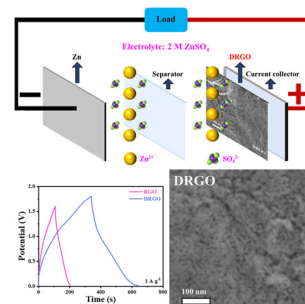
Sourav Dey, Sarai Dery Folkestad, Alexander C. Paul, Henrik Koch and Anna I. Krylov*



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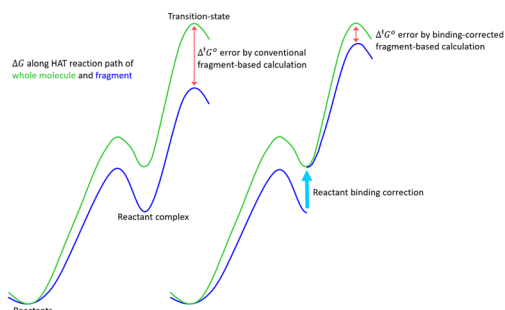
High-energy-density zinc ion capacitors based on 3D porous free-standing defect-reduced graphene oxide hydrogel cathodes

Peng Liao, Xiang Yu, Jiaqi He,* Xin Zhang, Wenjie Yan, Zenghui Qiu* and Haijun Xu*



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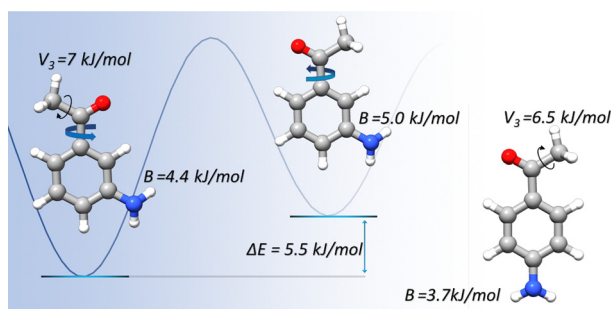
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Robust fragment-based method of calculating hydrogen atom transfer activation barrier in complex molecules

Yizhou Liu,* Frank C. Pickard IV, Gregory W. Sluggett and Iason G. Mustakis

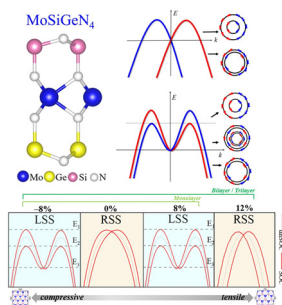
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Giovanna Salvitti, Silvia Sigismondi, Sonia Melandri, Juan Carlos López, Susana Blanco* and Assimo Maris*

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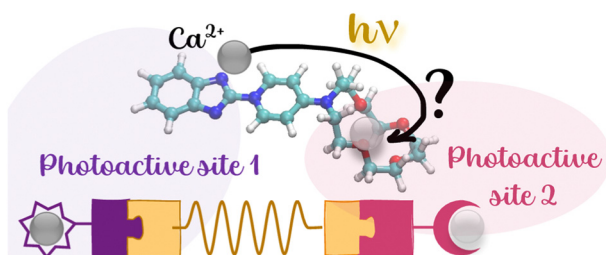


Biaxial strain modulated electronic structures of layered two-dimensional MoSiGeN₄ Rashba systems

Puxuan Li, Xuan Wang, Haoyu Wang, Qikun Tian, Jinyuan Xu, Linfeng Yu, Guangzhao Qin* and Zhenzhen Qin*

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In silico strategy to design an efficient organic photoswitch based on excited-state cation transfer

Laure de Thieulloy, Cédric Mongin, Isabelle Leray, Clément Guerrin, Guy Buntinx, Stéphane Aloïse and Aurélie Perrier*

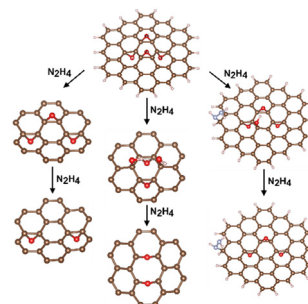


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Exploring the mechanism of graphene-oxide reduction by hydrazine in a multi-epoxide environment with DFT calculations

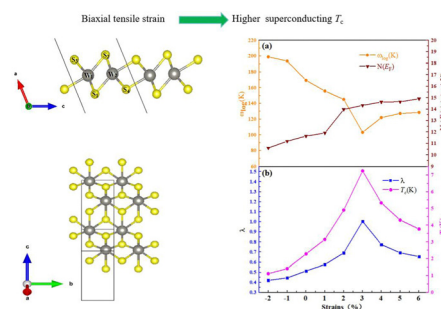
Nguyen Tri Hieu, Dénes Szieberth and Eszter Makkos*



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First-principles prediction of superconducting properties of monolayer 1T'-WS₂ under biaxial tensile strain

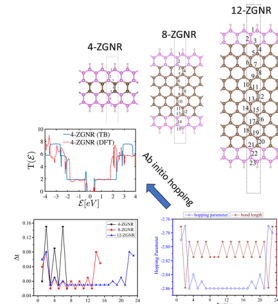
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1936

Influence of *ab initio* derived site-dependent hopping parameters on electronic transport in graphene nanoribbons

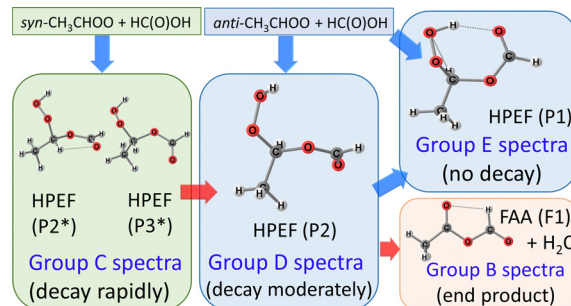
Masoumeh Davoudiniya, Bo Yang and Biplab Sanyal*



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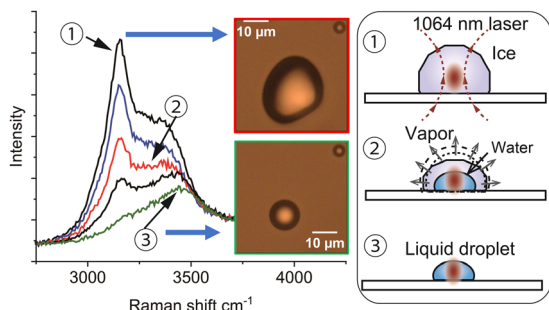
Detailed mechanism and kinetics of reactions of *anti*- and *syn*-CH₃CHOO with HC(O)OH: infrared spectra of conformers of hydroperoxyethyl formate

Bedabyas Behera and Yuan-Pern Lee*



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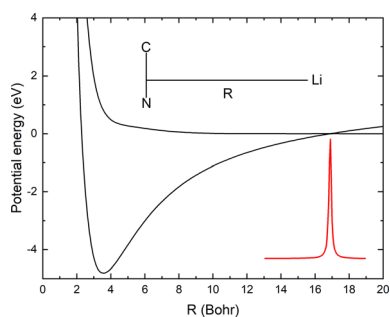
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Melting of a single ice microparticle on exposure to focused near-IR laser beam to yield a supercooled water droplet

Shuichi Hashimoto* and Takayuki Uwada

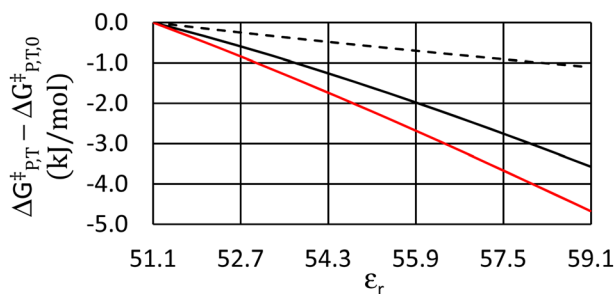
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Mutual neutralization in collisions of Li^+ with CN^-

Åsa Larson* and Ann E. Orel

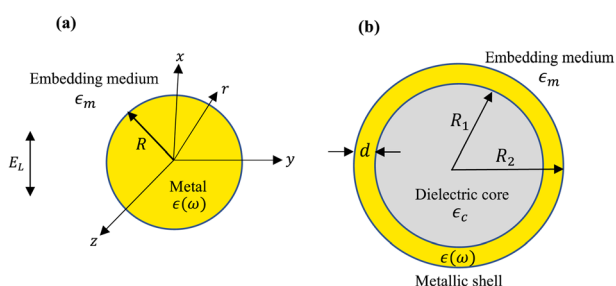
1984



A thermodynamic approach to analyzing relative permittivity and solvent mole fraction models, and application to $\text{S}_{\text{N}}1$ reactions

Floyd L. Wiseman* and Dane W. Scott

1994



Bandwidth of quantized surface plasmons: competition between radiative and nonradiative damping effects

Samar Moustafa, Mohamed K. Zayed, Moustafa Ahmed and Hesham Fares*

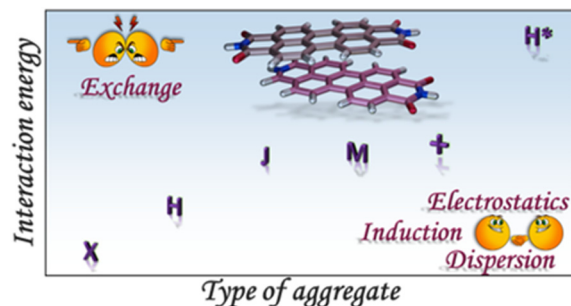


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2007

Energy landscape of perylenediimide chromophoric aggregates

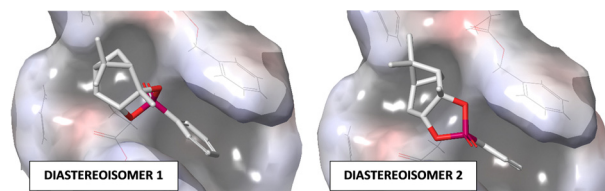
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Exploring the impact of alignment media on RDC analysis of phosphorus-containing compounds: a molecular docking approach

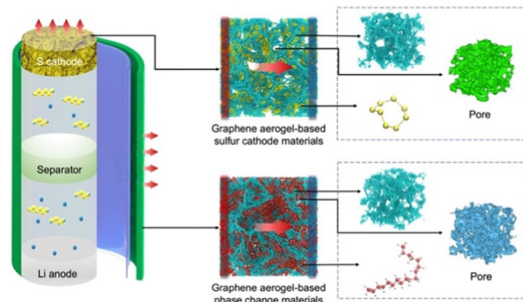
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Thermal transport properties of graphene aerogel as an advanced carrier for enhanced energy storage

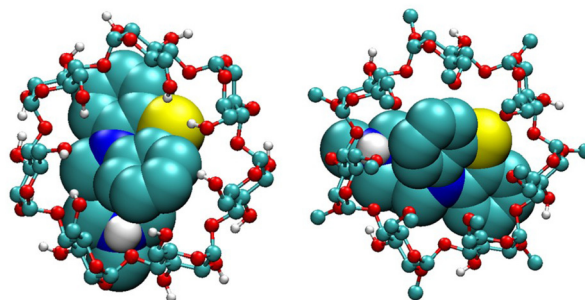
Jieren Song,* Xianghua Xu and Xingang Liang



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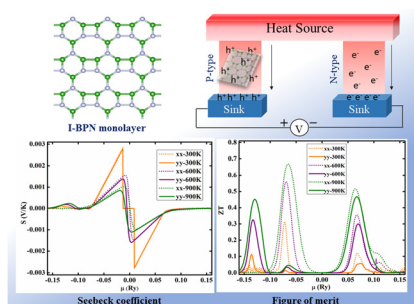
Host–guest systems for the SAMPL9 blinded prediction challenge: phenothiazine as a privileged scaffold for binding to cyclodextrins

Brenda Andrade, Ashley Chen and Michael K. Gilson*



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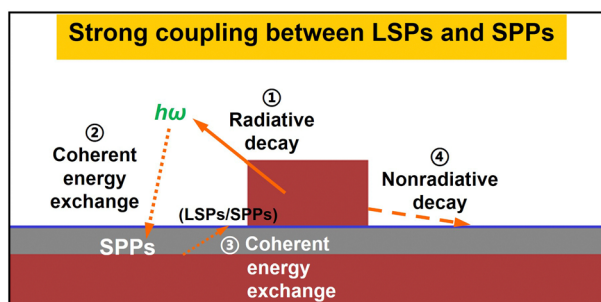
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Theoretical insights into the structural, electronic and thermoelectric properties of the inorganic biphenylene monolayer

Ajay Kumar, Parbati Senapati and Prakash Parida*

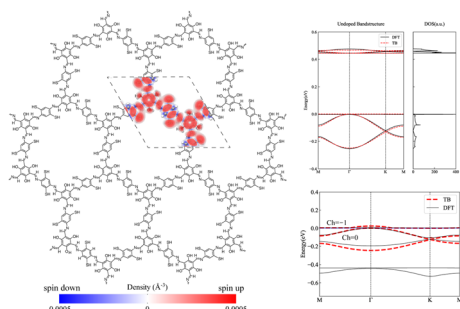
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Tailoring linear and nonlinear plasmons of metal/MoS₂/metal nanostructures

Shuangqing Jiang, Zonglin Li, Jingwu Tang,*
Wen Huang, Zanzian Tan, Dingyu Pan, Xiyang Chen and
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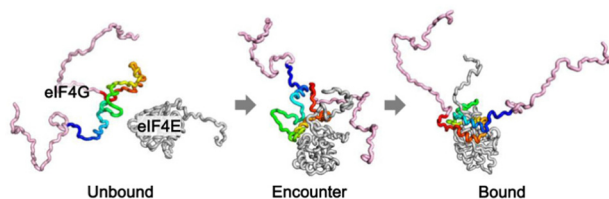
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Enantiomorphous kagome bands in a two-dimensional covalent organic framework with non-trivial magnetic and topological properties

Quan Gao, Xuelian Sun, Xuhui Xu, Xinxin Jiang,
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Desheng Liu*

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Molecular dynamics simulations revealed topological frustration in the binding-wrapping process of eIF4G with eIF4E

Meng Gao and Yongqi Huang*

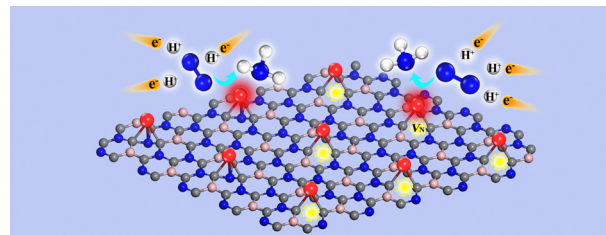


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Nitrogen-vacancy-modulated efficient ammonia desorption over 3d TM-anchored BC₃N₂ monolayer

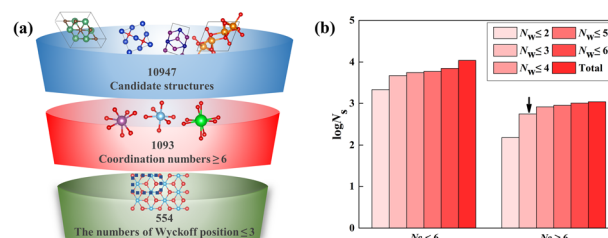
Long Lin, Kun Xie and Chaozheng He*



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High-throughput computational materials screening of transition metal peroxides

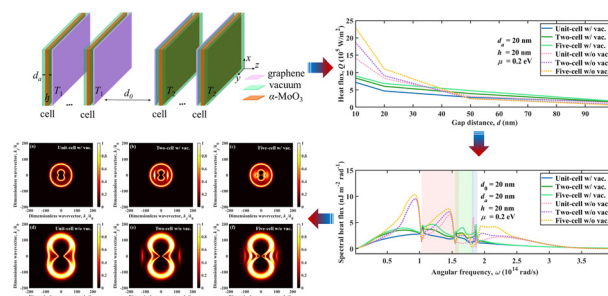
Yin-Hui Peng, Chang-Chun He, Yu-Jun Zhao and Xiao-Bao Yang*



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Coupling polaritons in near-field radiative heat transfer between multilayer graphene/vacuum/ α -MoO₃/vacuum heterostructures

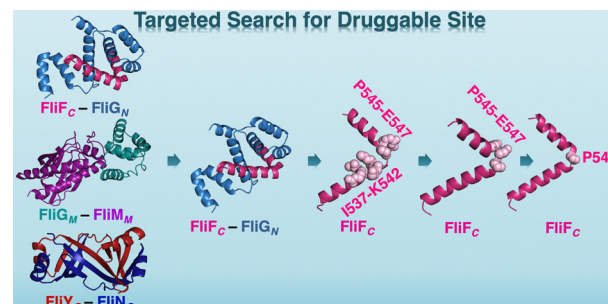
Jihong Zhang, Xiaohu Wu,* Yang Hu, Bing Yang, Haotuo Liu and Qilin Cai*



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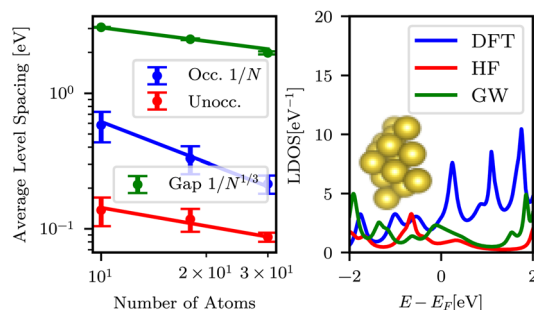
Flagellar motor protein-targeted search for the druggable site of *Helicobacter pylori*

Vaishnavi Tammara, Ruchika Angrover, Disha Sirur and Atanu Das*



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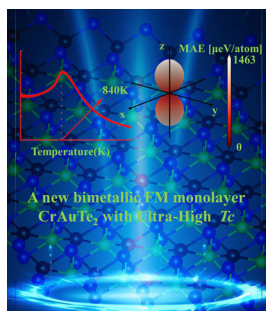
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Widening of the fundamental gap in cluster GW for metal–molecular interfaces

Štěpán Marek* and Richard Korytár

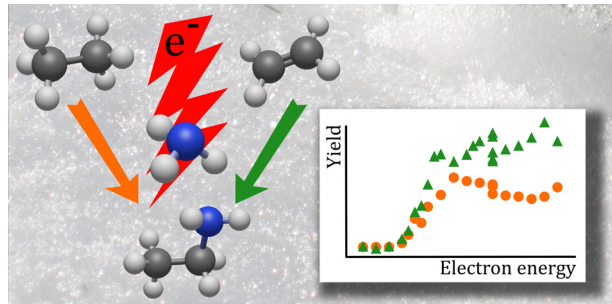
2134



Toward intrinsic ultra-high-temperature ferromagnetism in a CrAuTe₂/graphene heterosystem

Chaobin Jia, Chao Jin, Puyuan Shi, Jingjuan Su, Yungeng Zhang,* Xianghong Niu* and Bing Wang*

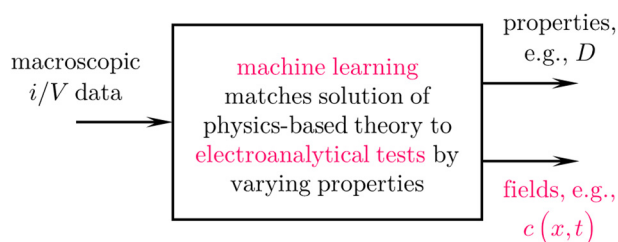
2140



Electron-induced hydroamination of ethane as compared to ethene: implications for the reaction mechanism

Hannah Boeckers, Martin Philipp Mues, Jan Hendrik Bredehöft and Petra Swiderek*

2153



How machine learning can extend electroanalytical measurements beyond analytical interpretation

Aashutosh Mistry,* Ian D. Johnson, Jordi Cabana, Brian J. Ingram* and Venkat Srinivasan*

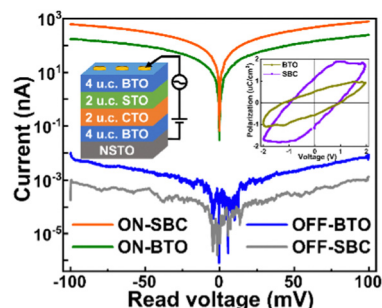


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2168

Giant tunnel resistance effect in $(\text{SrTiO}_3)_2/(\text{BaTiO}_3)_4/(\text{CaTiO}_3)_2$ asymmetric superlattice with enhanced polarization

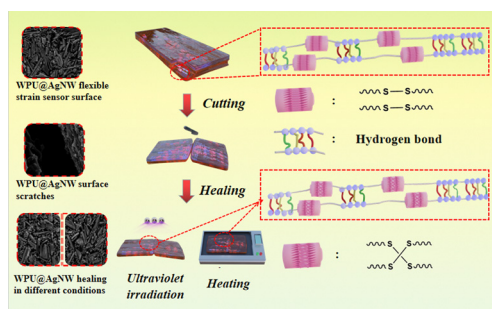
Xiubing Zhang, Haoming Wei,* Yangqing Wu, Tengzhou Yang and Bingqiang Cao*



2175

Multifunctional aqueous polyurethanes with high strength and self-healing efficiency based on silver nanowires for flexible strain sensors

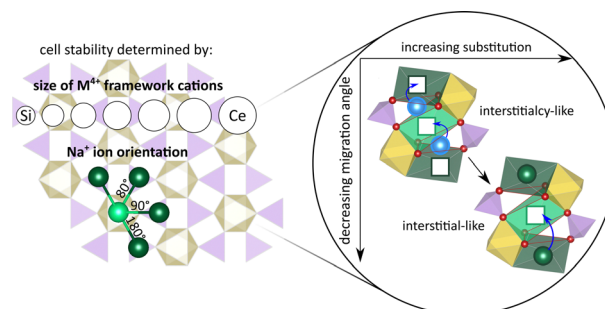
Haibin Niu, Jiaqi Li, Xin Song, Kaiyang Zhao, Li Liu,* Chao Zhou and Guangfeng Wu*



2190

Interstitial or interstitialcy: effect of the cation size on the migration mechanism in NaSiCON materials

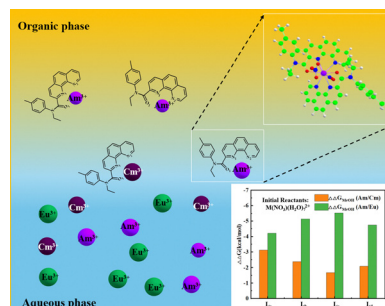
Judith Schuett, Johanna Schillings and Steffen Neitzel-Grieshammer*



2205

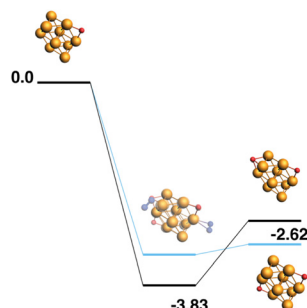
Theoretical investigations into the bonding and separation properties of non-rigid, partially rigid, and rigid ligands derived from Et-Tol-PTA with trivalent lanthanides and actinides

Shouqiang Wu and An Yong Li*



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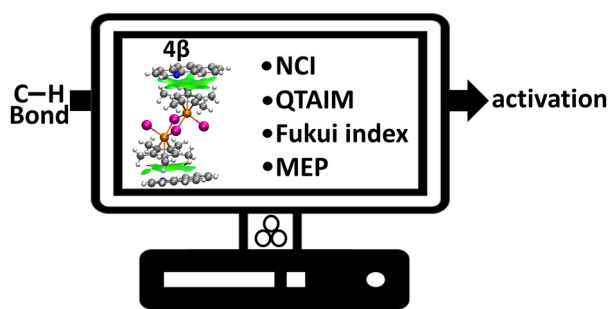
2218



Reactions of N_2O and CO on neutral Rh_{10}O_n clusters: a density functional study

Vikram Muman, Alex Tennyson-Davies, Oihan Allegret and Matthew A. Addicoat*

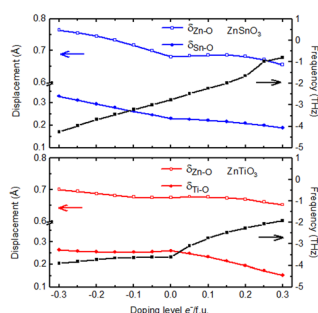
2228



Interactions and reactivity in crystalline intermediates of mechanochemical cyclorhodation reactions

Sara Gómez,* Santiago Gómez, Natalia Rojas-Valencia, José G. Hernández, Karen J. Ardila-Fierro, Tatiana Gómez, Carlos Cárdenas, Cacier Hadad, Chiara Cappelli and Albeiro Restrepo*

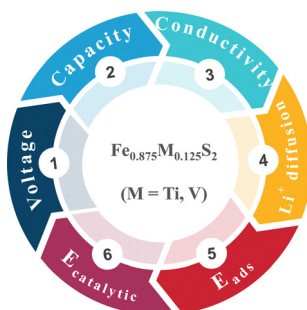
2242



Comparison of carrier doping in ZnSnO_3 and ZnTiO_3 from first principles

Jing Li, Jing Su, Qing Zhang, Changfeng Fang* and Xiaohui Liu*

2249



First-principles study of the discharge electrochemical and catalytic performance of the sulfur cathode host $\text{Fe}_{0.875}\text{M}_{0.125}\text{S}_2$ ($\text{M} = \text{Ti}, \text{V}$)

Cheng-Dong Wei, Hong-Tao Xue, Yu-Xia Hu, Qing-Shan Zhao and Fu-Ling Tang*

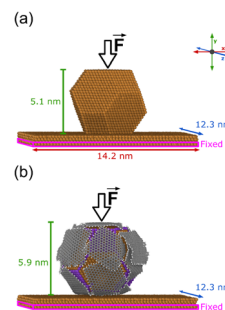


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2260

On the mechanical response of graphene-capped copper nanoparticles

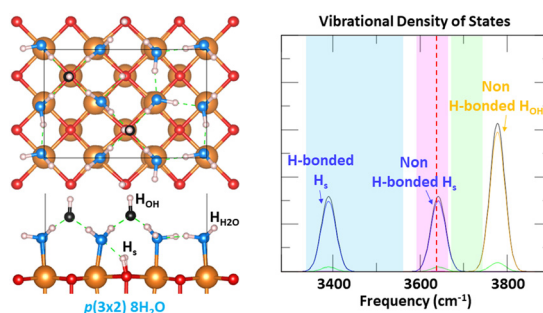
Gabriel J. Olguín-Orellana, Juan A. de la Rosa Abad, Maria B. Camarada, Sergio J. Mejía-Rosales, Jans Alzate-Morales and Marcelo M. Mariscal*



2269

First principles simulations of MgO(100) surface hydration at ambient conditions

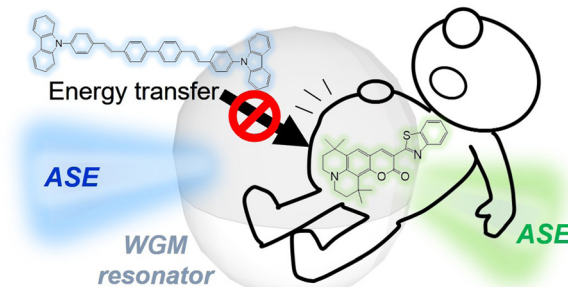
Michel Sassi* and Kevin M. Rosso



2277

Device parameter to evaluate exciton energy transfer in organic whispering-gallery-mode microresonators and its dependence on the amplified spontaneous emission threshold

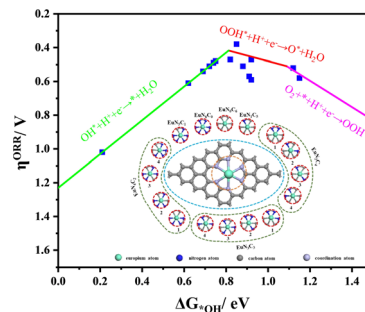
Tomoki Mikajiri, Takeshi Komino,* Jun-ichi Yamada and Hiroyuki Tajima



2284

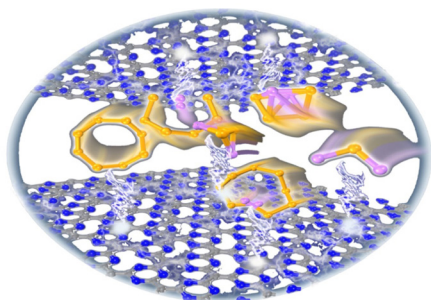
Mechanistic study of Eu single atoms occupying four vacancy centers as potential electrocatalysts for the oxygen reduction reaction

Qiming Fu, Daomiao Wang* and Chao Liu*



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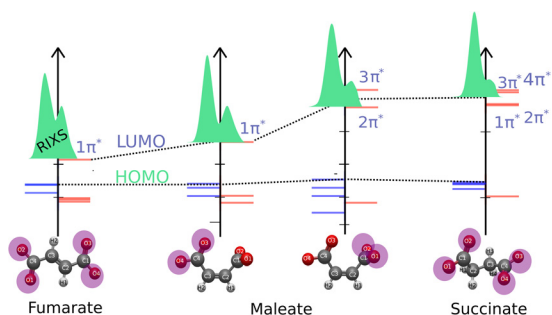
2291



Anchoring and catalytic insights into bilayer C_4N_3 material for lithium–selenium batteries: a first-principles study

Zehui Yang, Wentao Liu, Shulin Bai, Peng Ai, Hao Wang, Tuo Zheng, Qingshun Li and Shuwei Tang*

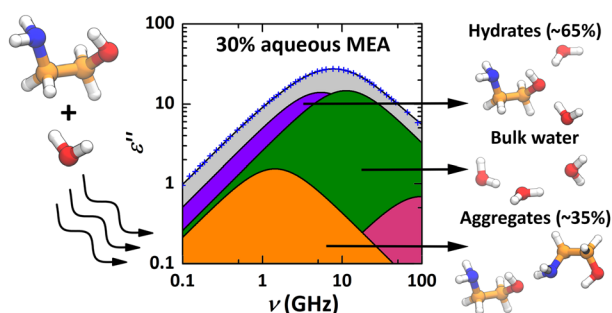
2304



Electronic structure, bonding and stability of fumarate, maleate, and succinate dianions from X-ray spectroscopy

Viktoriia Savchenko,* Sebastian Eckert, Mattis Fondell, Rolf Mitzner, Vincius Vaz da Cruz and Alexander Föhlisch

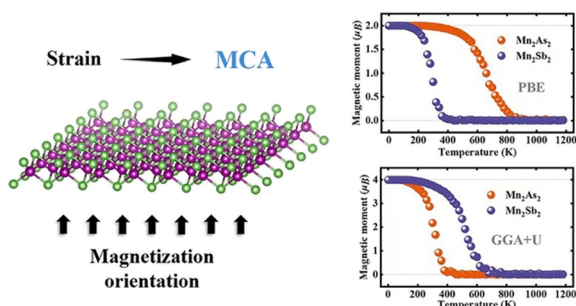
2312



What is behind a gas stream scrubbing liquid? Monoethanolamine/water mixtures as seen by dielectric relaxation spectroscopy

Vira Agjeienko* and Richard Buchner

2324



Theoretical prediction of two-dimensional ferromagnetic Mn_2X_2 ($X = As, Sb$) with strain-controlled magnetocrystalline anisotropy

Yi Zhao, Zesen Lei, Yonghao Wang, Wei Yan,* Ruishan Tan, Tao Jing and Qilong Sun*

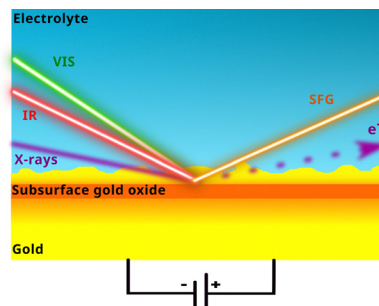


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2332

Multi-spectroscopic study of electrochemically-formed oxide-derived gold electrodes

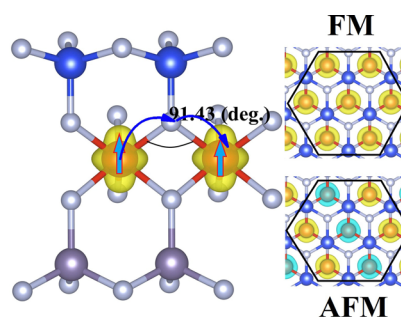
Sara Boscolo Bibi, Ahmed M. El-Zohry,*
Bernadette Davies, Vladimir Grigorev,
Christopher M. Goodwin, Patrick Lömker,
Alexander Holm, Harri Ali-Löytty,
Fernando Garcia-Martinez, Christoph Schlueter,
Markus Soldemo, Sergey Koroidov* and Tony Hansson*



2341

Tunable polarization properties of charge, spin, and valley in Janus VSiGeZ₄ (Z = N, P, As) monolayers

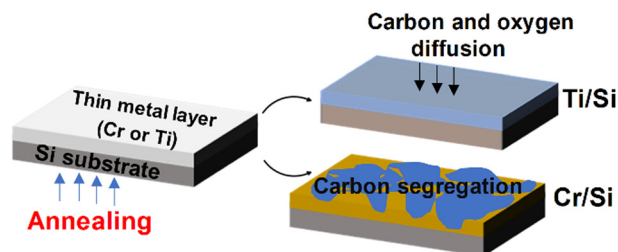
Ming-Yang Liu,* Guang-Qiang Li, Yao He and Kai Xiong



2355

Enhancing electrocatalytic activity in metallic thin films through surface segregation of carbon

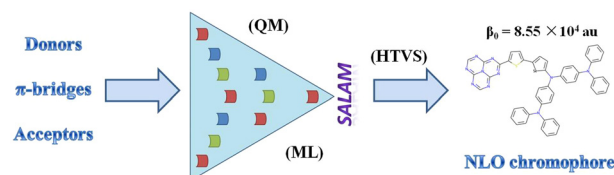
Ayesha Kousar, Ulviyya Quliyeva, Ishan Pande,
Jani Sainio, Jaakko Julin, Timo Sajavaara,
Antti J. Karttunen and Tomi Laurila*



2363

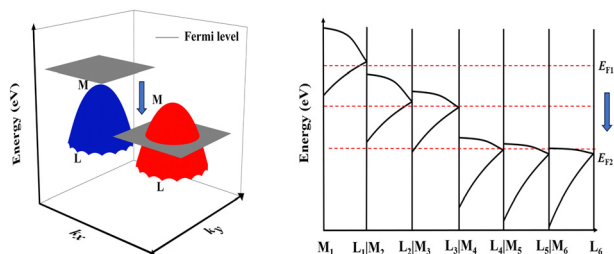
High-throughput virtual screening of organic second-order nonlinear optical chromophores within the donor- π -bridge-acceptor framework

Chunyun Tu,* Weijiang Huang, Sheng Liang, Kui Wang,
Qin Tian and Wei Yan*



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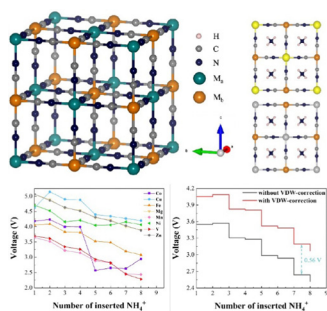
2376



Theoretical study of CDW phases for bulk NbX₂ (X = S and Se)

Hongwei Du, Zhenyi Jiang,* Jiming Zheng,*
Xiaodong Zhang, Wenxuan Wang and Zhiyong Zhang

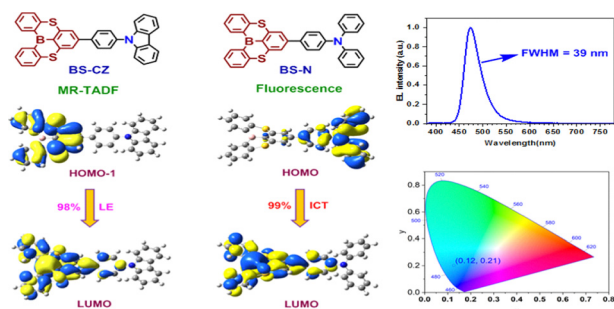
2387



Element screening of metal sites in Fe-based Prussian blue framework materials for ammonium ion battery applications: a first-principles study

Yu Zhang, Junjie Xing, Bo Zhang, Likai Tong and
Xiuli Fu*

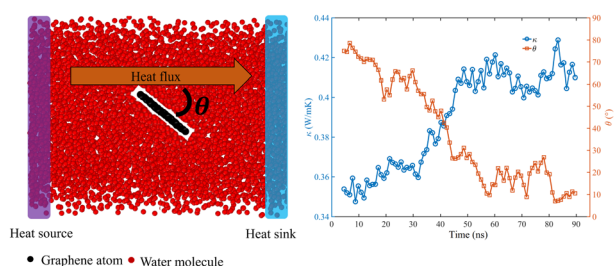
2395



B-embedded disulfide-bridged π -conjugated compounds: structures and optical tuning

Kaishun Ye, Gang Li, Feiyang Li, Chao Shi,* Zhen Jiang,
Fuzheng Zhang, Qiuxia Li,* Jie Su, Dandan Song* and
Aihua Yuan

2402



Coupling at the molecular scale between the graphene nanosheet and water and its effect on the thermal conductivity of the nanofluid

Xiong Pan, Hanhui Jin,* Xiaoke Ku, Yu Guo and
Jianren Fan

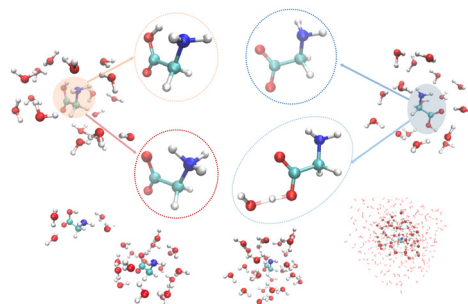


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2414

Temperature driven transformations of glycine molecules embedded in interstellar ice

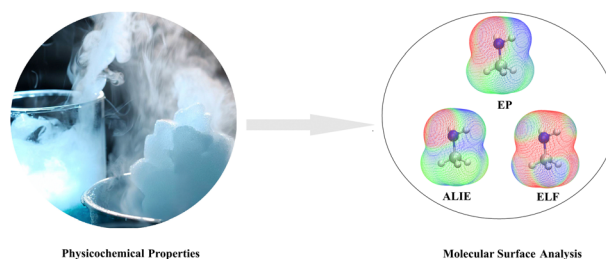
Maysa Yusef-Buey, Tzonka Mineva, Dahbia Talbi and Mathias Rapacioli*



2426

Boiling, critical, and freezing temperatures in light of molecular descriptors: correlation and causation

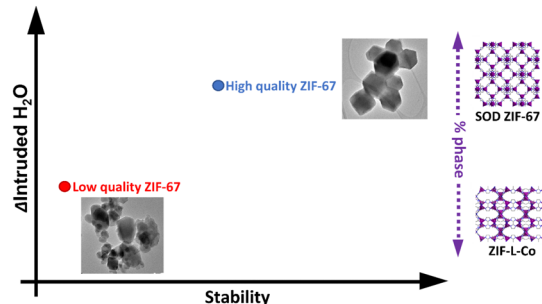
Ossama Abdeen, Mohamed Ismael* and Aly Abdou*



2440

Quality-dependent performance of hydrophobic ZIF-67 upon high-pressure water intrusion–extrusion process

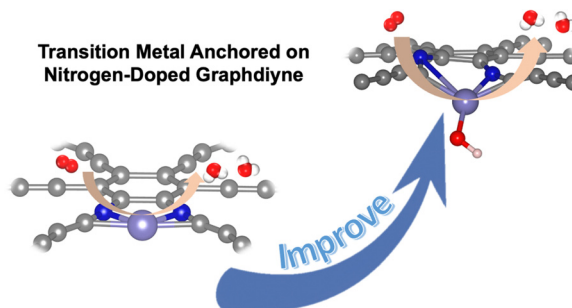
Eder Amayuelas,* Luis Bartolomé, Yan Zhang, Juan Miguel López del Amo, Oleksandr Bondarchuk, Artem Nikulin, Francisco Bonilla, Elena Palomo del Barrio, Paweł Zajdel* and Yaroslav Grosu*



2449

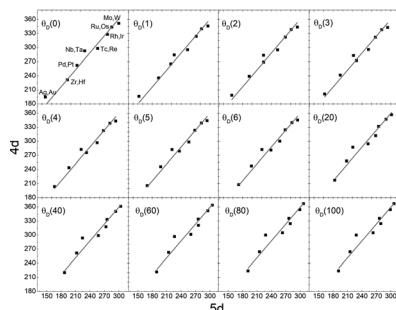
Transition metals anchored on nitrogen-doped graphdiyne for an efficient oxygen reduction reaction: a DFT study

Ning Wang, Siyu Gan, Yunfeng Mao, Junping Xiao,* Chunming Xu and Tianhang Zhou*



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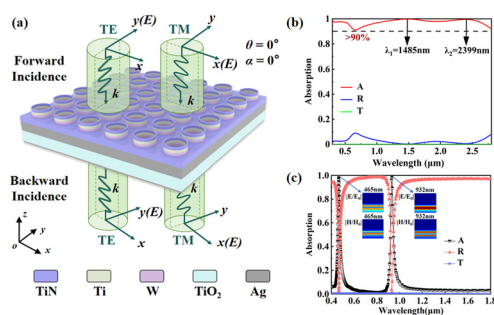
2457



Vibrational and cohesive properties in 4d and 5d transition metals: systematics and interrelations

Dalia S. Bertoldi* and A. Fernández Guillermet

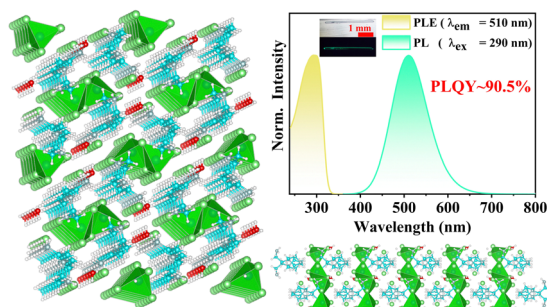
2463



A multifunctional switching bidirectional optical absorber based on a titanium nitride metamaterial

Lijing Su, Hengli Feng, Pengfei Sun, Yaxin Zhou, Xin Li, Sihan Nie, Lingling Ran and Yang Gao*

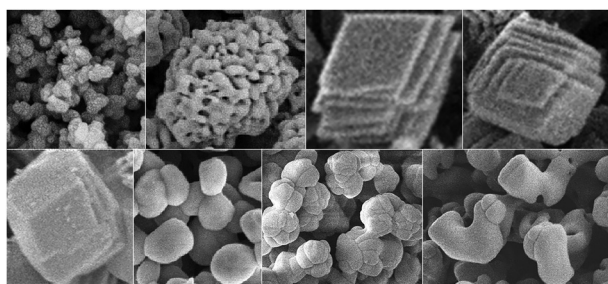
2472



A zero-dimensional hybrid copper(I) bromide single crystal with highly efficient green emission

Yingui Gao, Zhihuang Xu, Liwang Ye, Yuanjie Wang and Xinxin Zhuang*

2478



Morphologies and magnetic properties of α -Fe₂O₃ nanoparticles calcined at different temperatures

Xue-Min He, Duan-Qing Chen, Kun-Yu Su, Zhen-Fei Yu, Yi Zhang and Wei Zhong*

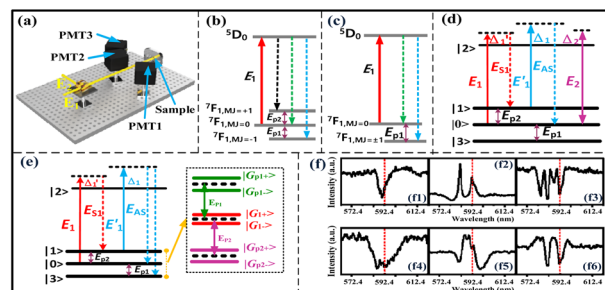


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2486

Spectral and temporal atomic coherence interaction in $\text{Eu}^{3+}:\text{NaYF}_4$ and $\text{Eu}^{3+}:\text{BiPO}_4$

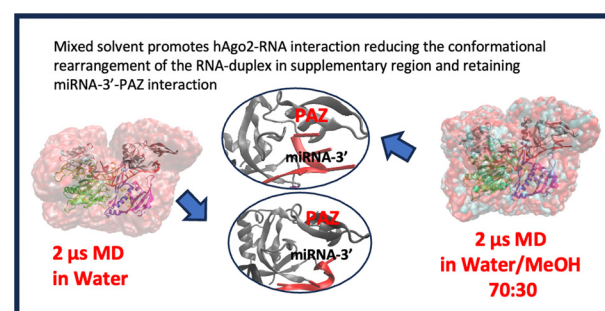
Zhou Feng, Muhammad Imran, Faisal Nadeem, Huanrong Fan, Jin Yan, Irfan Ahmed, Condon Lau* and Yanpeng Zhang*



2497

Probing the conformational dynamics of an Ago–RNA complex in water/methanol solution

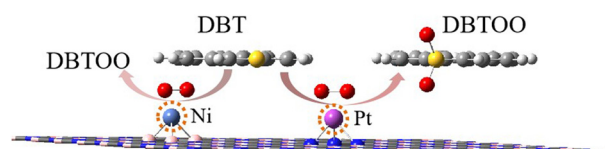
Francesco Porcelli, Anna Rita Casavola, Alessandro Grottesi, Donatella Schiumarini and Lorenzo Avaldi



2509

The single metal atom (Ni, Pd, Pt) anchored on defective hexagonal boron nitride for oxidative desulfurization

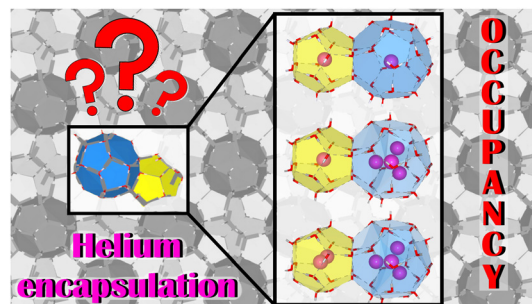
Naixia Lv, Hongshun Ran, Jinrui Zhang, Jie Yin, Yuan Zhang, Hongping Li* and Linhua Zhu*



2519

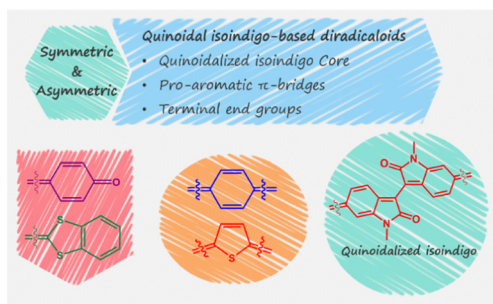
Analysing the stability of He-filled hydrates: how many He atoms fit in the sII crystal?

Raquel Yanes-Rodríguez and Rita Prosmiti*



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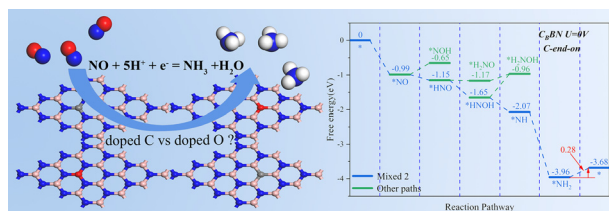
2529



Sufficient driving force for quinoidal isoindigo-based diradicaloids with tunable diradical characters

Li Shen,* Xiaobo Gao, Zhanqing Chang, Changhao Zhang, Yue Li, Jitao Lu, Qingguo Meng and Qian Wu*

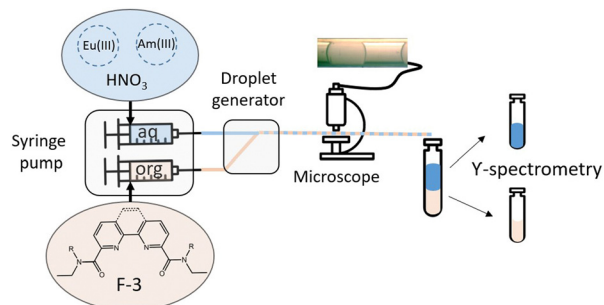
2539



Carbon doped hexagonal boron nitride as an efficient metal-free catalyst for NO capture and reduction

Jiali Nie, Ying Li, Dongyue Gao, Yi Fang, Jing Lin, Chengchun Tang and Zhonglu Guo*

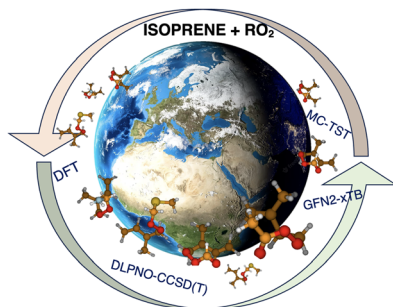
2548



Kinetic features of solvent extraction by N,O-donor ligands of f-elements: a comparative study of diamides based on 1,10-phenanthroline and 2,2'-bipyridine

Ekaterina A. Konopkina,* Alexander V. Gopin, Anton S. Pozdeev, Maria G. Chernysheva, Paulina Kalle, Elizaveta A. Pavlova, Stepan N. Kalmykov, Vladimir G. Petrov, Nataliya E. Borisova, Alexander A. Guda and Petr I. Matveev

2560



Cost-effective approach for atmospheric accretion reactions: a case of peroxy radical addition to isoprene

Dominika Pasik, Siddharth Iyer and Nanna Myllys*

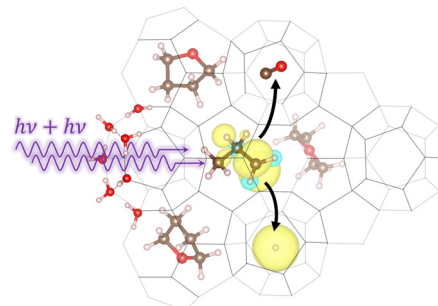


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Two-photon chemistry of tetrahydrofuran in clathrate hydrates

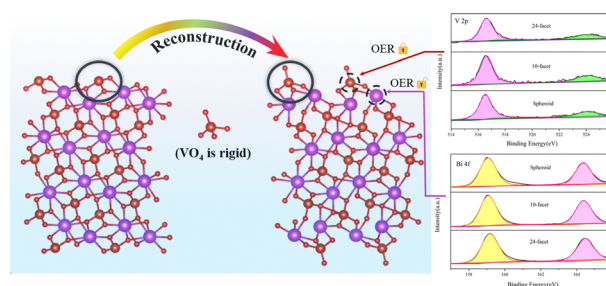
Michael A. Michon,* Pawel Chmielniak, Peter M. Weber* and Christoph Rose-Petruck*



2580

Oxygen evolution reaction (OER) active sites in BiVO₄ studied using density functional theory and XPS experiments

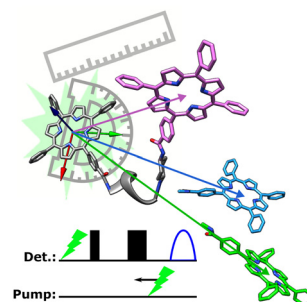
Qingyan Zhang, Guowei Liu and Taifeng Liu*



2589

Determining and controlling conformational information from orientationally selective light-induced triplet–triplet electron resonance spectroscopy for a set of bis-porphyrin rulers

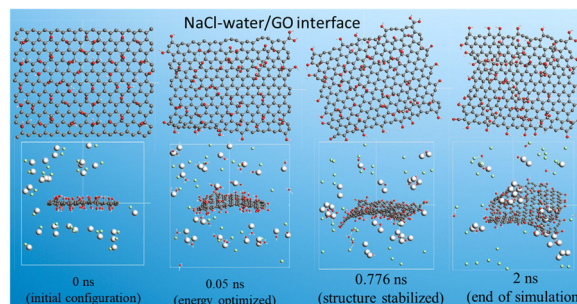
Arnau Bertran,* Marta De Zotti, Christiane R. Timmel, Marilena Di Valentin* and Alice M. Bowen*



2603

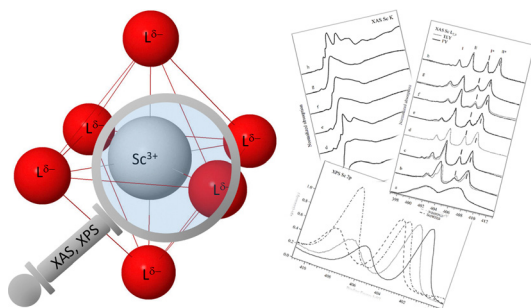
ReaxFF molecular dynamics of graphene oxide/NaCl aqueous solution interfaces

Rokhsareh Akbarzadeh and Milan Predota*



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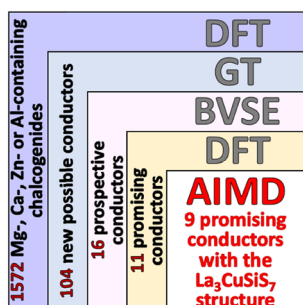
2613



Chemical bonding effects in Sc compounds studied using X-ray absorption and X-ray photoelectron spectroscopies

Anna Zimina,* Aline Léon and Ralph Steininger

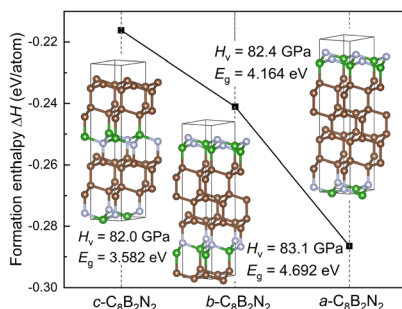
2622



A novel class of multivalent ionic conductors with the $\text{La}_3\text{CuSiS}_7$ structure type: results of stepwise ICSD screening

Artem A. Kabanov,* Yelizaveta A. Morkhova,* Vladislav T. Osipov, Manuel Rothenberger, Tilmann Leisegang and Vladislav A. Blatov

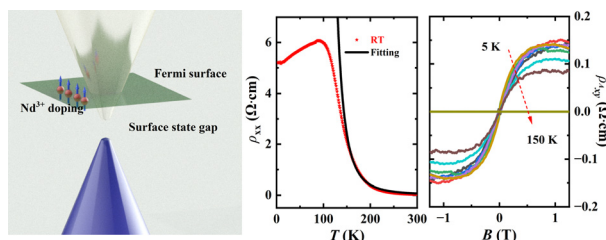
2629



Novel superhard semiconducting structures of $\text{C}_8\text{B}_2\text{N}_2$ predicted using the first-principles approach

Xiao-Wei Sun,* Meng-Ru Chen, Ting Song, Jun-Hong Tian, Zi-Jiang Liu and Wen-Chao Huang

2638



Anomalous Hall effect in Nd-doped $\text{Bi}_{1.1}\text{Sb}_{0.9}\text{STe}_2$ topological insulator single crystals

Lei Chen, Weiyao Zhao, Kaijian Xing, Mengyun You, Xiaolin Wang and Ren-Kui Zheng*

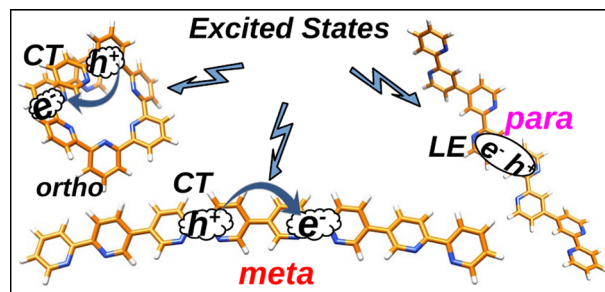


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Contrasting the excited state properties of different conformers of *trans*- and *cis*-2,2'-bipyridine oligomers in the gas phase

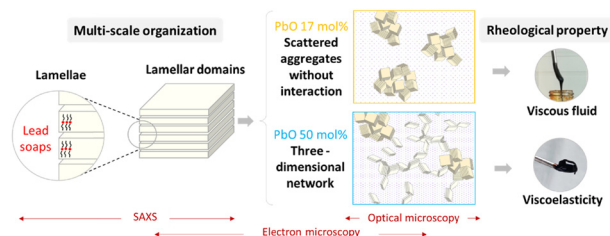
Palak Mandal and Aditya N. Panda*



2657

Multiscale organisation of lead carboxylates in artistic oil binders

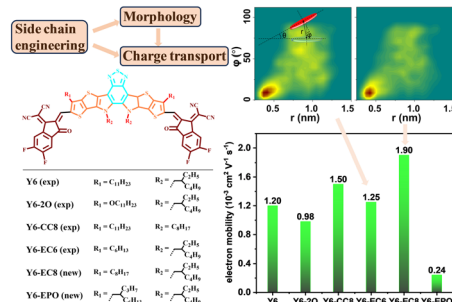
Lucie Laporte, Frédéric Gobeaux, Thierry Pouget, Nicolas Benoot, Julien Foison, David Touboul, Guylaine Ducouret and Laurence de Viguerie*



2666

The effects of side chain engineering on the morphology and charge transport of the A-DA₁D-A type of non-fullerene acceptor: a multiscale study

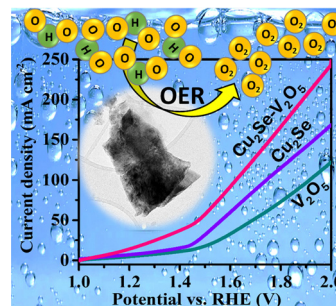
Zhijun Cao and Shaohui Zheng*



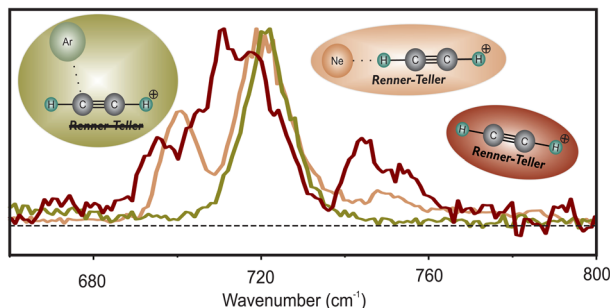
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Synergistic effect of a bamboo-like Bi₂S₃ covered Sm₂O₃ nanocomposite (Bi₂S₃-Sm₂O₃) for enhanced alkaline OER

Tauseef Munawar, Saman Fatima, Khalid Mujasam Batoo, Ambreen Bashir, Faisal Mukhtar, Sajjad Hussain, Sumaira Manzoor, Muhammad Naeem Ashiq, Shoukat Alim Khan, Muammer Koc and Faisal Iqbal*



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Leak-out spectroscopy as alternative method to rare-gas tagging for the Renner–Teller perturbed HCCH^+ and DCCD^+ ions

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