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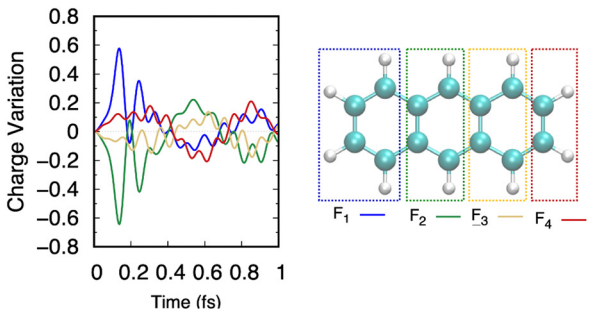
See Mathias Rapacioli *et al.*, pp. 1499–1515. Image reproduced by permission of Mathias Rapacioli and CNRS-5626 from *Phys. Chem. Chem. Phys.*, 2024, **26**, 1499.

REVIEWS

1499

Addressing electronic and dynamical evolution of molecules and molecular clusters: DFTB simulations of energy relaxation in polycyclic aromatic hydrocarbons

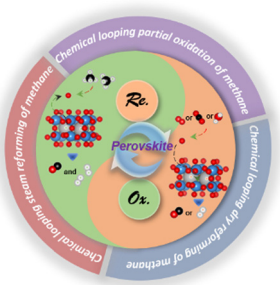
Mathias Rapacioli,* Maysa Yusef Buey and Fernand Spiegelman



1516

Perovskites as oxygen storage materials for chemical looping partial oxidation and reforming of methane

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



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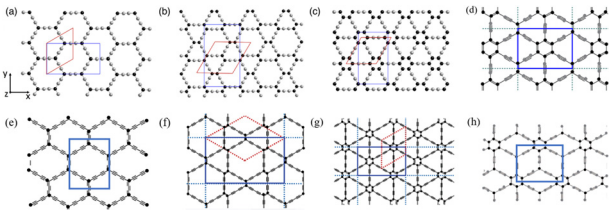
REVIEWS

1541

Graphyne and graphdiyne nanoribbons: from their structures and properties to potential applications

Qiaohan Liu, Xiaorong Wang, Jing Yu* and Jingang Wang*

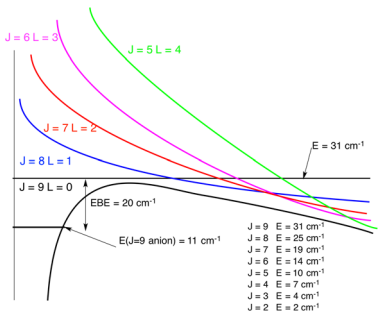


PERSPECTIVES

1564

An environmental impact statement for molecular anions

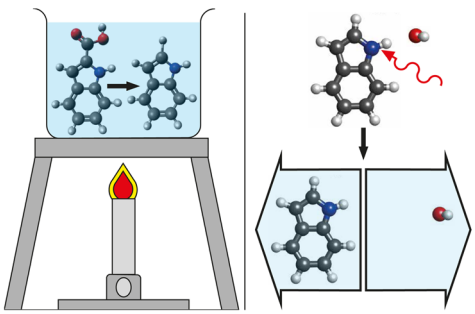
Jack Simons



1587

Unraveling the ultrafast dynamics of thermal-energy chemical reactions

Matthew S. Robinson and Jochen Küpper*

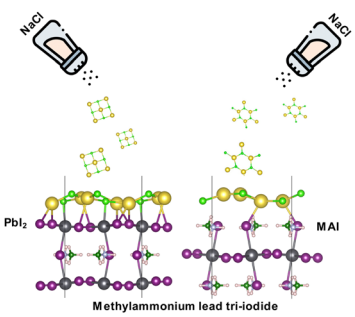


COMMUNICATIONS

1602

Exotic hexagonal NaCl atom-thin layer on methylammonium lead iodide perovskite: new hints for perovskite solar cells from first-principles calculations

Adriana Pecoraro, Ana B. Muñoz-García,* Gennaro V. Sannino, Paola Delli Veneri and Michele Pavone*



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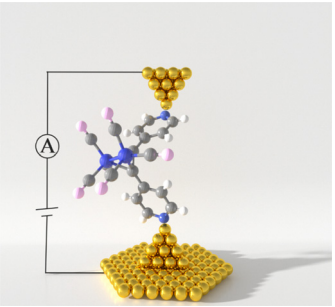
COMMUNICATIONS

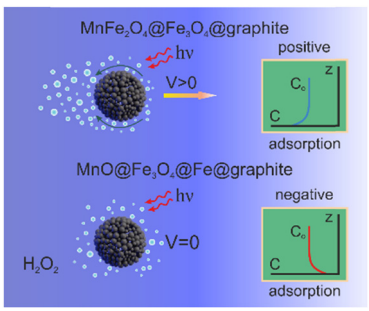
1608



Manipulating the charge transport *via* incorporating a cobalt bridge into a single-molecule junction

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

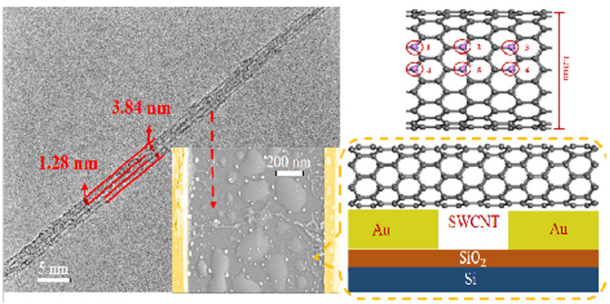
1612



The role of self-diffusiophoresis and reactive force during the propulsion of manganese-based catalytic micromotors

Boris Kichatov,* Alexey Korshunov, Vladimir Sudakov, Alexandr Golubkov, Dmitriy Smovzh,* Salavat Sakhapov and Mikhail Skirda

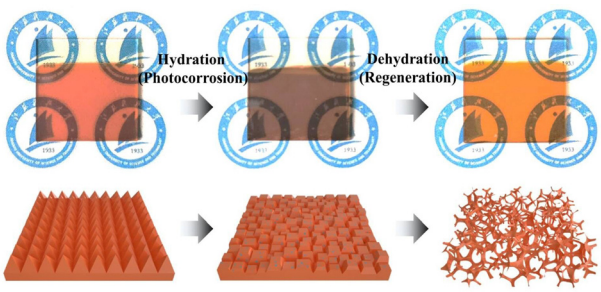
1616



Single walled carbon nanotubes band gap width measurement and the influence of nitrogen doping research

Rui Miao, Yujian Liang, Guangfeng Zhou, Yayu Deng, Lei Wang, Jingui Deng and Qingyi Shao*

1625



Hydration deactivation mechanism of the ⟨100⟩ oriented cuprous oxide photocathodes in solar water splitting and the regenerated three-dimensional structure

Yang Li,* Jiating Wu, Yuhe Zheng, Yajing Fan, Ting Bian, Xinyu Fan, Santana Vimbai Masendu, Junhua Xu and Zongping Shao*

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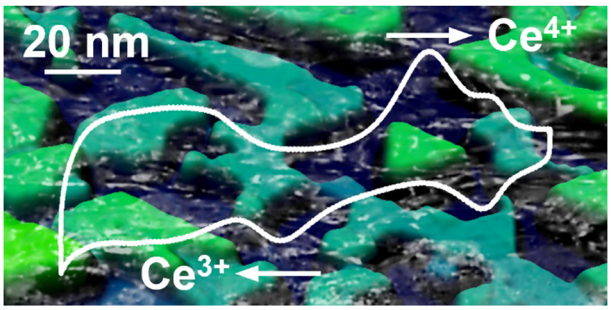
RESEARCH PAPERS

1630

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

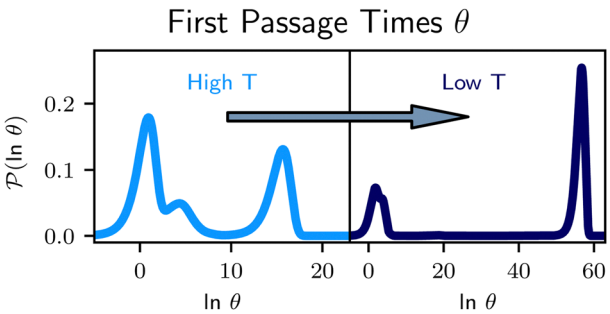
Lukáš Fusek, Pankaj Kumar Samal, Jiří Keresteš, Ivan Khalakhan, Viktor Johánek, Yaroslava Lykhach, Jörg Libuda, Olaf Brummel* and Josef Mysliveček*



1640

Analysis and interpretation of first passage time distributions featuring rare events

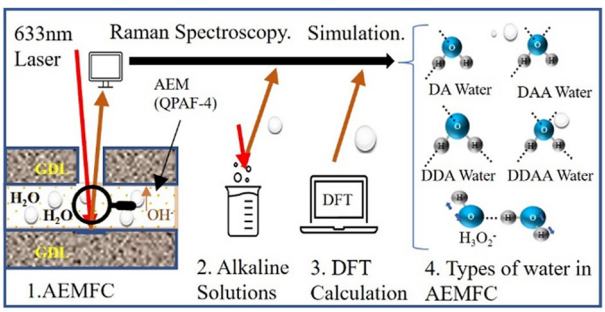
Esmae J. Woods and David J. Wales*



1658

Various states of water species in an anion exchange membrane characterized by Raman spectroscopy under controlled temperature and humidity

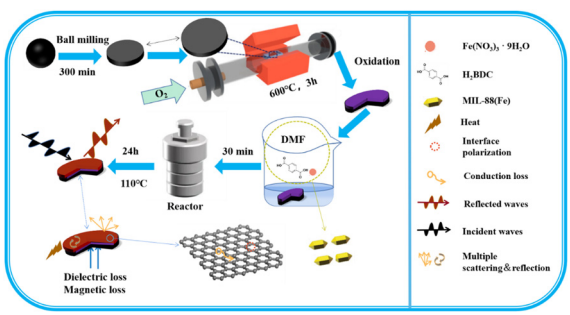
Solomon Wekesa Wakolo, Donald A. Tryk, Hiromichi Nishiyama, Kenji Miyatake, Akihiro Iiyama and Junji Inukai*



1671

Preparation of MIL-88(Fe)@Fe_2O_3@FeSiCr double core–shell-structural composites and their wave-absorbing properties

Wenmiao Zhang, Hongzhang Du, Lei Wang,* Sajjad Ur Rehman, Shuqi Shen, Weiwei Dong, Yifeng Hu, Haiping Zou* and Tongxiang Liang



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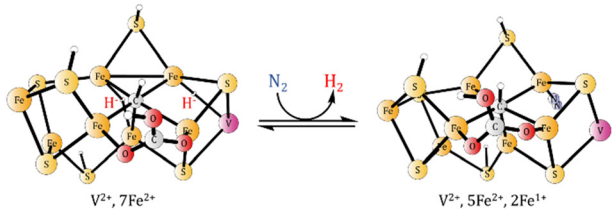
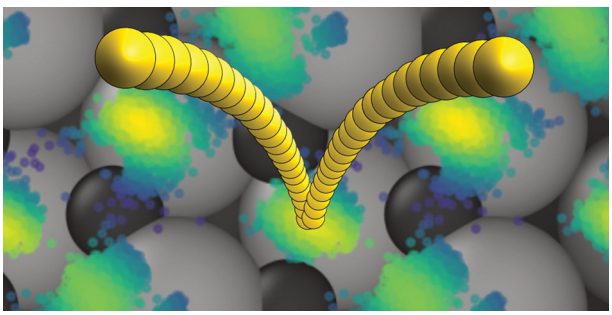


The energetics of N_2 reduction by vanadium containing nitrogenase

Per E. M. Siegbahn* and Wen-Jie Wei

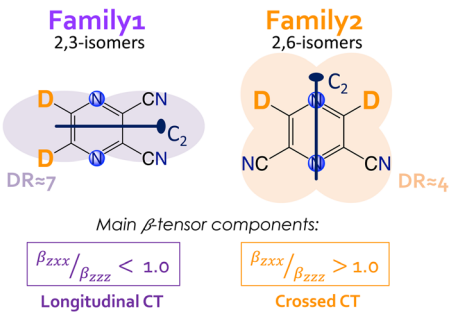
1696



Hydrogen atom scattering at the Al_2O_3(0001) surface: a combined experimental and theoretical study

Martin Liebetrau, Yvonne Dorenkamp, Oliver Bünermann* and Jörg Behler*

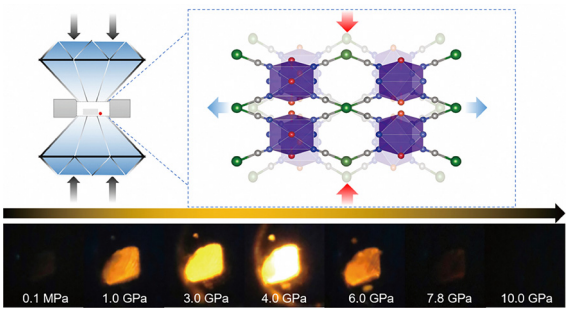
1709



Second-order nonlinear optical properties of X-shaped pyrazine derivatives

Verònica Postils,* Zuzana Burešová, David Casanova, Benoît Champagne, Filip Bureš, Vincent Rodriguez* and Frédéric Castet*

1722



Negative linear compressibility and strong enhancement of emission in $Eu[Ag(CN)_2]_3 \cdot 3H_2O$ under pressure

Yu Liu, Boyang Fu, Min Wu, Weilong He, Donghua Liu,* Fuyang Liu, Luhong Wang, Haozhe Liu, Kai Wang and Weizhao Cai*

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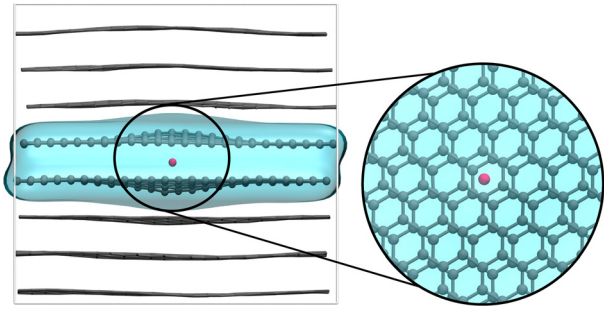
1729

Towards hybrid quantum mechanical/molecular mechanical simulations of Li and Na intercalation in graphite – force field development and DFTB parametrisation

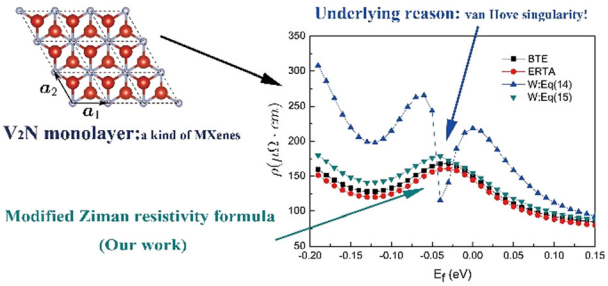
Felix R. S. Purtscher and Thomas S. Hofer*



1741

First-principles calculations on the intrinsic resistivity of realistic metals: a case study of monolayer V_2N

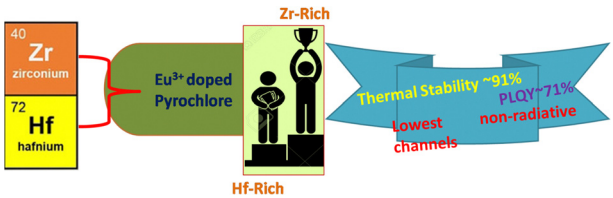
Binyuan Zhang and Weijiang Gong*



1749

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

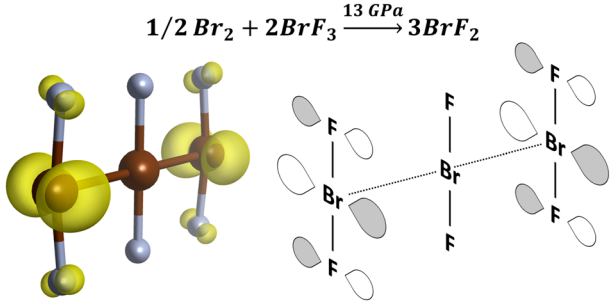
Santosh K. Gupta,* Sandeep Nigam and Yuanbing Mao



1762

High-pressure stabilization of open–shell bromine fluorides

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



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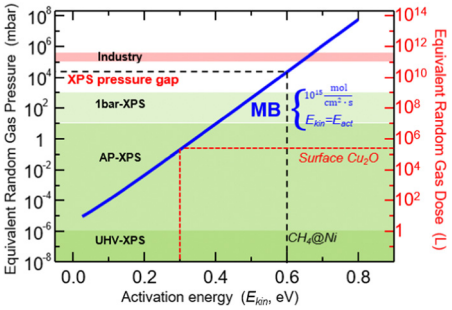
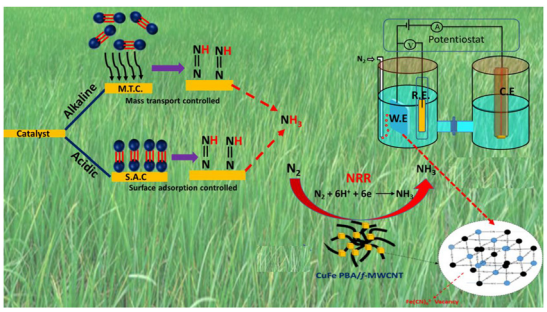


Simulating high-pressure surface reactions with molecular beams

Amjad Al Taleb, Frederik Schiller, Denis V. Vyalikh, José María Pérez, Sabine V. Auras, Daniel Farías and J. Enrique Ortega*

1777



Mechanistic insights into the electrolyte effects on the electrochemical nitrogen reduction reaction using copper hexacyanoferrate/f-MWCNT nano-composites

Aamir Y. Bhat, Priya Jain, Mohsin A. Bhat and Pravin P. Ingole*

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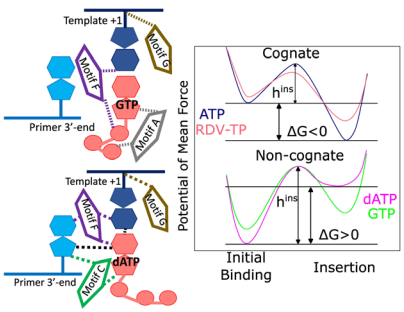
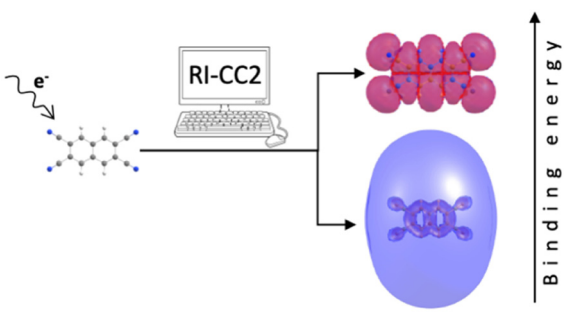


Trapping a non-cognate nucleotide upon initial binding for replication fidelity control in SARS-CoV-2 RNA dependent RNA polymerase

Moises E. Romero, Shannon J. McElhenney and Jin Yu*

1809



On the performance of second-order approximate coupled-cluster singles and doubles methods for non-valence anions

Garrette Pauley Paran, Cansu Utku and Thomas-Christian Jagau*

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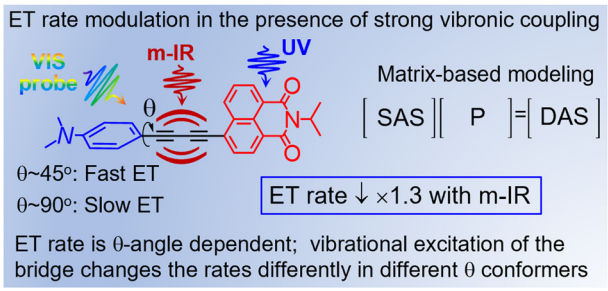
Electron transfer rate modulation with mid-IR in butadiyne-bridged donor–bridge–acceptor compounds

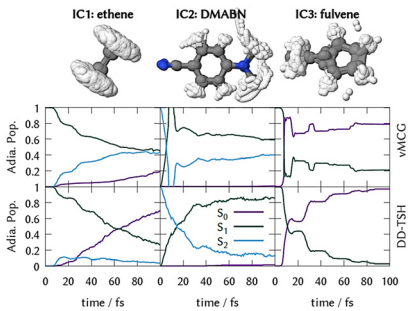
Kasun C. Mendis, Xiao Li, Jesús Valdiviezo, Susannah D. Banziger, Peng Zhang, Tong Ren, David N. Beratan and Igor V. Rubtsov*



1829

Benchmarking non-adiabatic quantum dynamics using the molecular Tully models

Sandra Gómez, Eryn Spinlove and Graham Worth*



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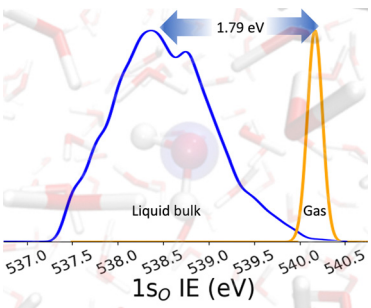
Core-ionization spectrum of liquid water

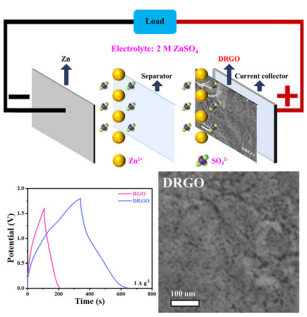
Sourav Dey, Sarai Dery Folkestad, Alexander C. Paul, Henrik Koch and Anna I. Krylov*



1860

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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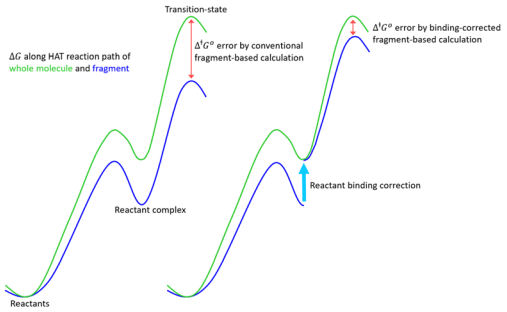
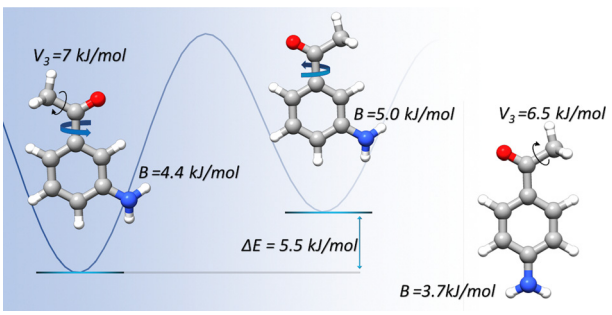


Robust fragment-based method of calculating hydrogen atom transfer activation barrier in complex molecules

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

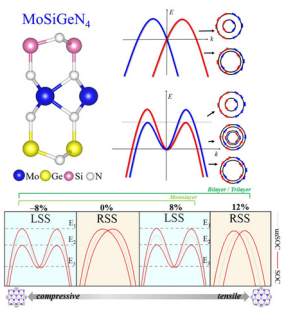
1881



Structure and dynamics of 3′-aminoacetophenone and 4′-aminoacetophenone from rotational spectroscopy

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

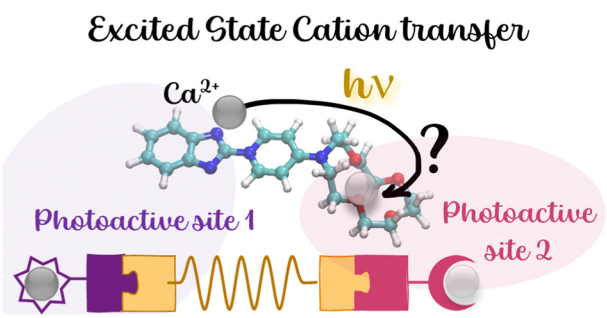
1891



Biaxial strain modulated electronic structures of layered two-dimensional $MoSiGeN_4$ Rashba systems

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

1904



***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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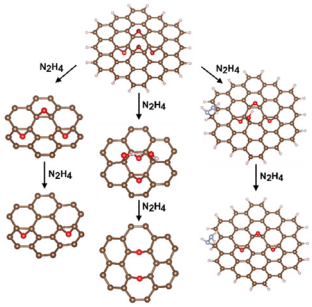
RESEARCH PAPERS

1917

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

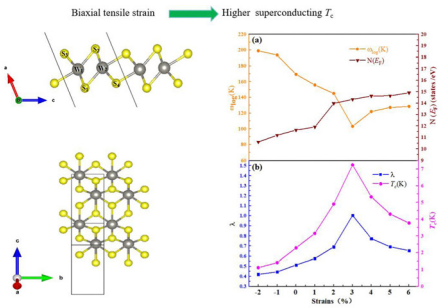
Nguyen Tri Hieu, Dénes Szieberth and Eszter Makkos*



1929

First-principles prediction of superconducting properties of monolayer 1T′-WS_2 under biaxial tensile strain

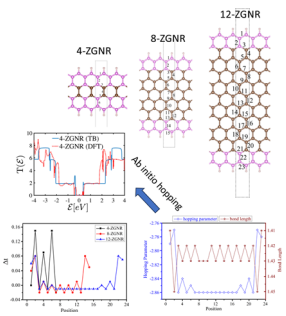
Guo-Hua Liu, Shu-Xiang Qiao, Qiu-Hao Wang, Hao Wang, Hao-Dong Liu, Xin-Zhu Yin, Jin-Han Tan, Na Jiao, Hong-Yan Lu* and Ping Zhang*



1936

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

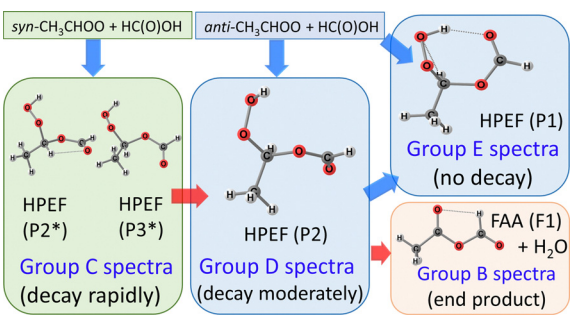
Masoumeh Davoudiniya, Bo Yang and Biplab Sanyal*



1950

Detailed mechanism and kinetics of reactions of *anti*- and *syn*-CH_3CHOO with HC(O)OH: infrared spectra of conformers of hydroperoxyethyl formate

Bedabyas Behera and Yuan-Pern Lee*



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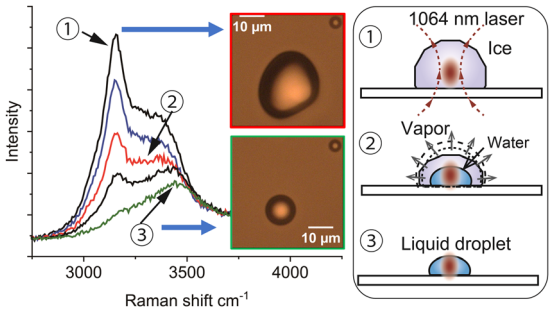
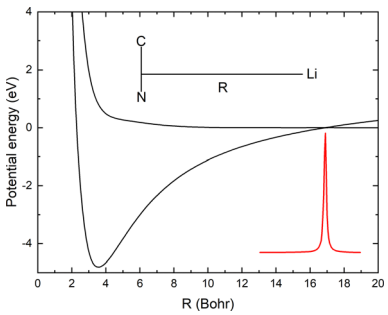
1967



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

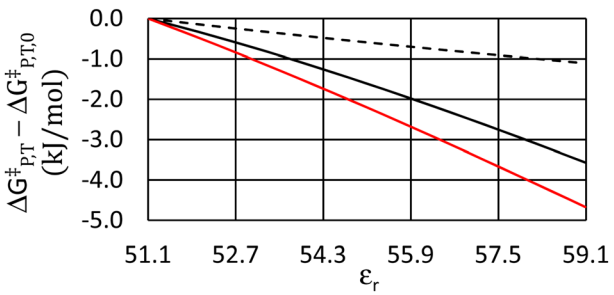
1977



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

Åsa Larson* and Ann E. Orel

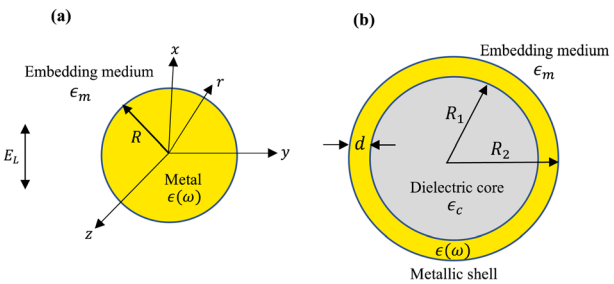
1984



A thermodynamic approach to analyzing relative permittivity and solvent mole fraction models, and application to S_N1 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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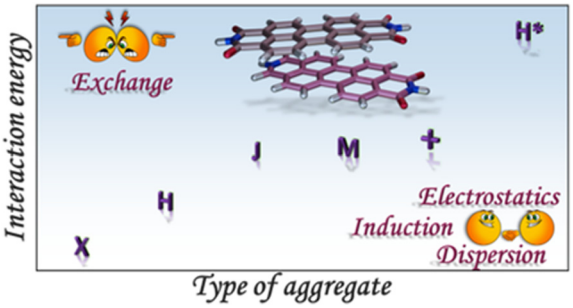
2007

Energy landscape of perylenediimide chromophoric aggregates

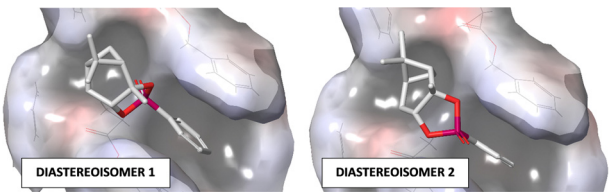
Pallavi Panthakkal Das, Aniruddha Mazumder, Megha Rajeevan, Rotti Srinivasamurthy Swathi* and Mahesh Hariharan*



2016

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

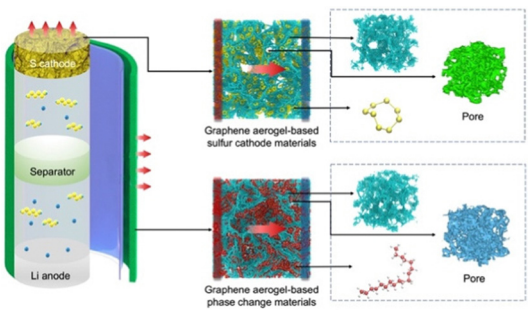
Markéta Christou Tichotová, Lucie Tučková, Hugo Kocek, Aleš Růžička, Michal Straka and Eliška Procházková*



2025

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

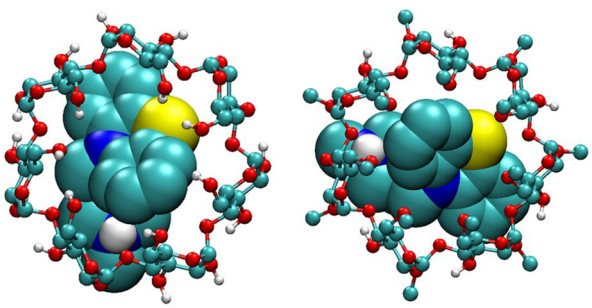
Jieren Song,* Xianghua Xu and Xingang Liang



2035

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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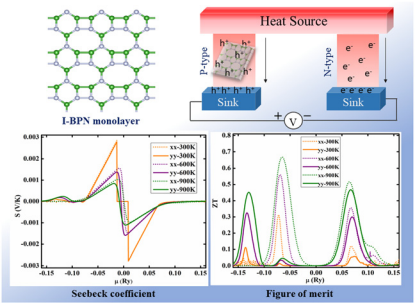
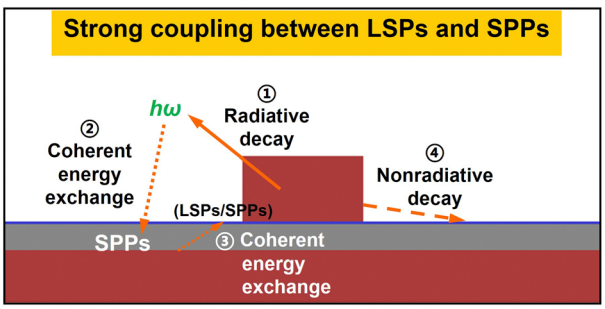
2044



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

Ajay Kumar, Parbati Senapati and Prakash Parida*

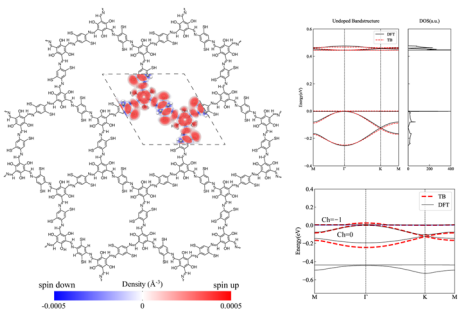
2058



Tailoring linear and nonlinear plasmons of metal/MoS_2/metal nanostructures

Shuangqing Jiang, Zonglin Li, Jingwu Tang,* Wen Huang, Zanxian Tan, Dingyu Pan, Xiyang Chen and Guozheng Nie*

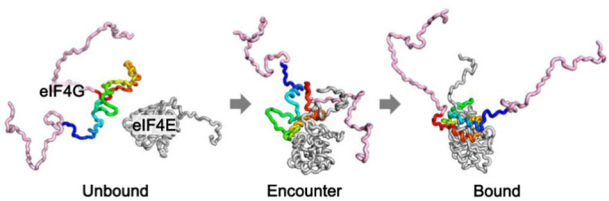
2066



Enantiomorphic kagome bands in a two-dimensional covalent organic framework with non-trivial magnetic and topological properties

Quan Gao, Xuelian Sun, Xuhui Xu, Xinxin Jiang, Zhikuan Wang, Lei Yang, Dongmei Li, Bin Cui* and Desheng Liu*

2073



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

Meng Gao and Yongqi Huang*

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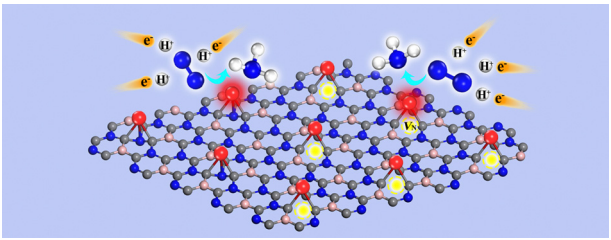
2082

Nitrogen-vacancy-modulated efficient ammonia desorption over 3d TM-anchored BC_3N_2 monolayer

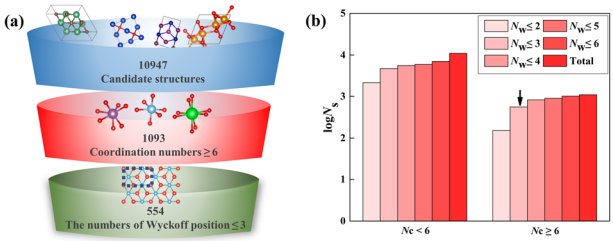
Long Lin, Kun Xie and Chaozheng He*



2093

High-throughput computational materials screening of transition metal peroxides

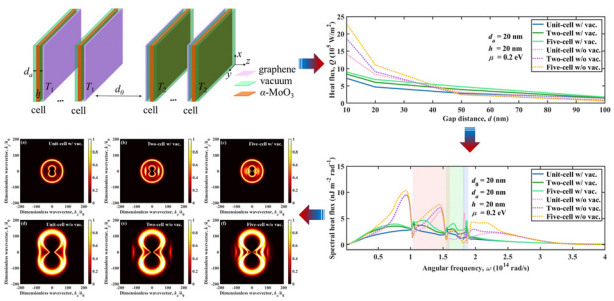
Yin-Hui Peng, Chang-Chun He, Yu-Jun Zhao and Xiao-Bao Yang*



2101

Coupling polaritons in near-field radiative heat transfer between multilayer graphene/vacuum/α-MoO_3/vacuum heterostructures

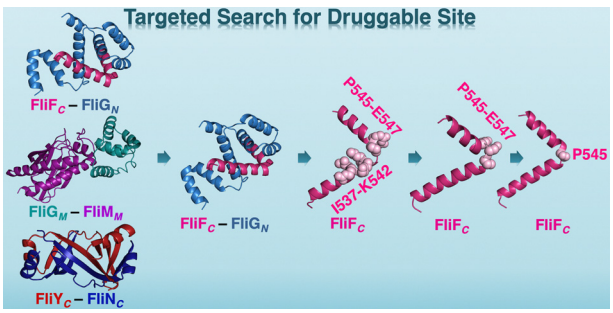
Jihong Zhang, Xiaohu Wu,* Yang Hu, Bing Yang, Haotuo Liu and Qilin Cai*



2111

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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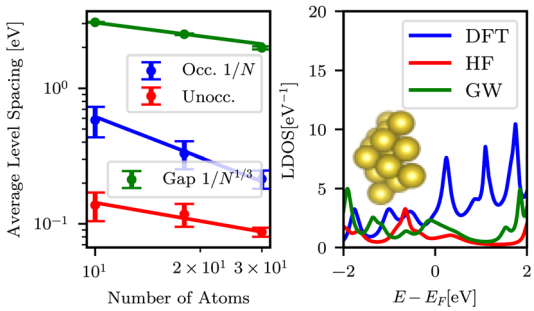
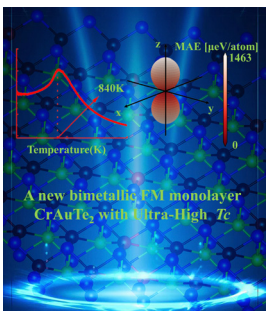
2127



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

Štěpán Marek* and Richard Korytár

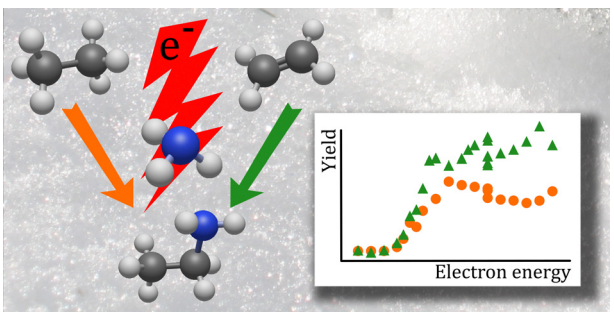
2134



Toward intrinsic ultra-high-temperature ferromagnetism in a $CrAuTe_2$/graphene heterosystem

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

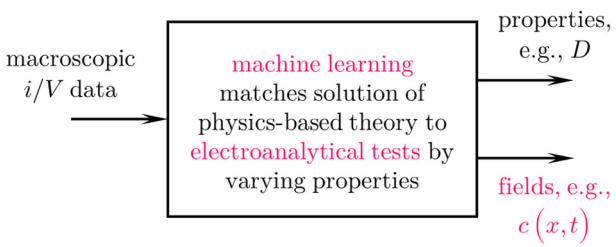
2140



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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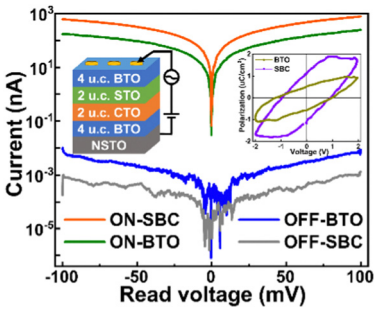
2168

Giant tunnel resistance effect in $(SrTiO_3)_2/(BaTiO_3)_4/(CaTiO_3)_2$ asymmetric superlattice with enhanced polarization

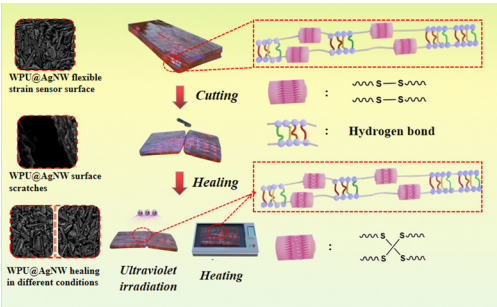
Xiubing Zhang, Haoming Wei,* Yangqing Wu, Tengzhou Yang and Bingqiang Cao*



2175

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

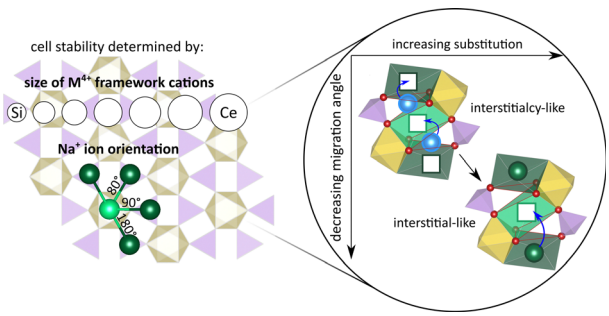
Haibin Niu, Jiaqi Li, Xin Song, Kaiyang Zhao, Li Liu,* Chao Zhou and Guangfeng Wu*



2190

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

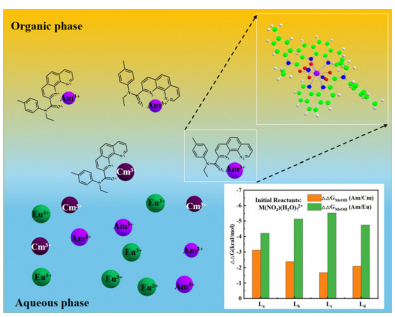
Judith Schuett, Johanna Schillings and Steffen Neitzel-Grieshammer*



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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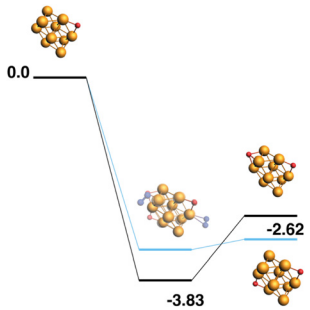
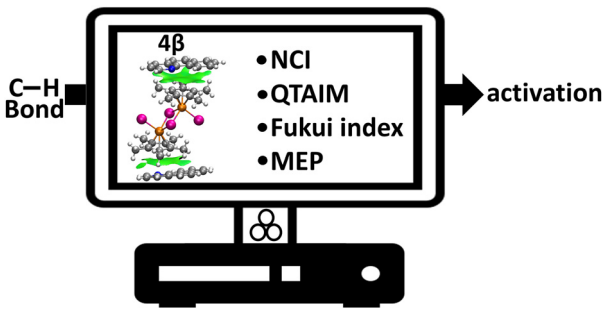
2218



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*

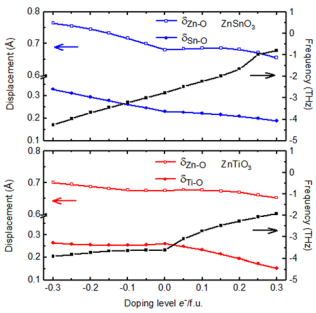
2228



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*

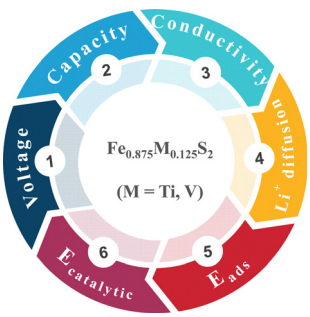
2242



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 $Fe_{0.875}M_{0.125}S_2$ (M = Ti, V)

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

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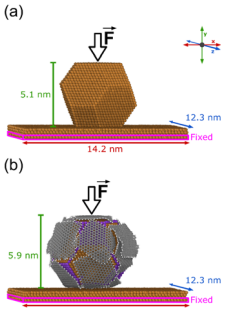
2260

On the mechanical response of graphene-capped copper nanoparticles

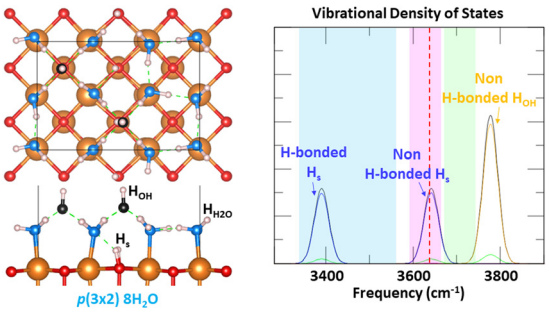
Gabriel J. Olguín-Orellana, Juan A. de la Rosa Abad, María B. Camarada, Sergio J. Mejía-Rosales, Jans Alzate-Morales and Marcelo M. Mariscal*



2269

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

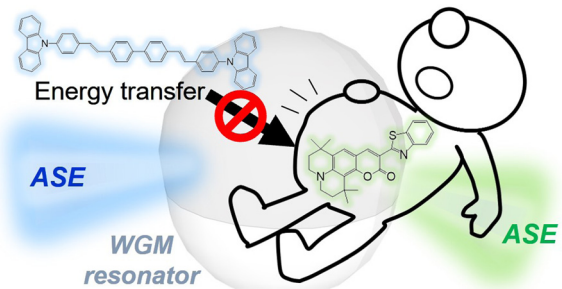
Michel Sassi* and Kevin M. Rosso



2277

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

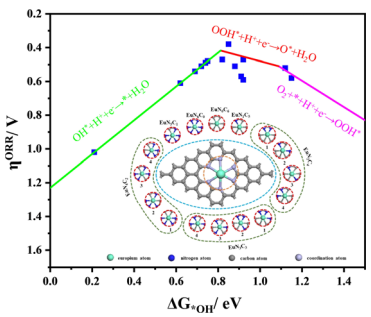
Tomoki Mikajiri, Takeshi Komino,* Jun-ichi Yamada and Hiroyuki Tajima



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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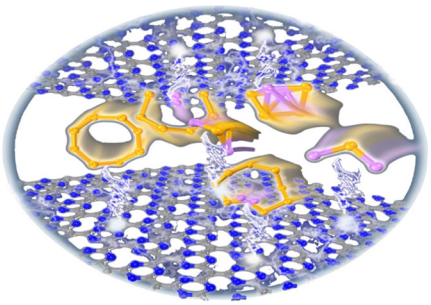
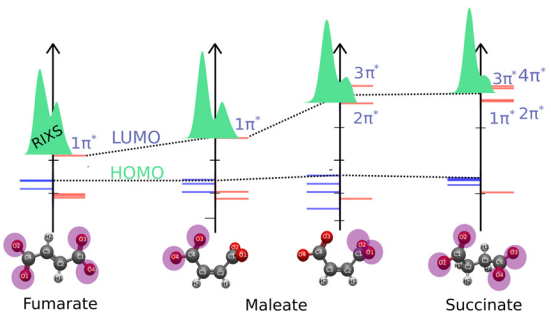


Anchoring and catalytic insights into bilayer C_4N_3 material for lithium–selenium batteries: a first-principles study

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

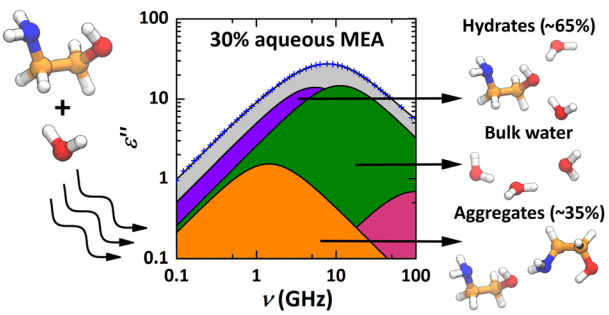
2304



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

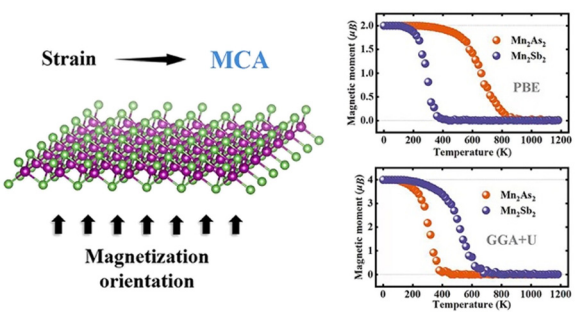
2312



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

Vira Agieienko* 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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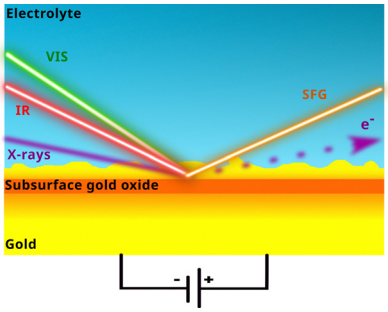
2332

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

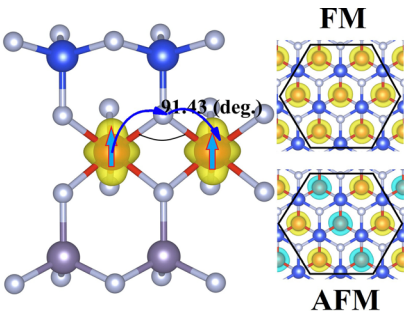
Sara Boscolo Bibi, Ahmed M. El-Zohry,* Bernadette Davies, Vladimir Grigorev, Christopher M. Goodwin, Patrick Lömker, Alexander Holm, Harri Ali-Löytty, Fernando Garcia-Martinez, Christoph Schlueter, Markus Soldemo, Sergey Koroidov* and Tony Hansson*



2341

Tunable polarization properties of charge, spin, and valley in Janus $VSiGeZ_4$ (Z = N, P, As) monolayers

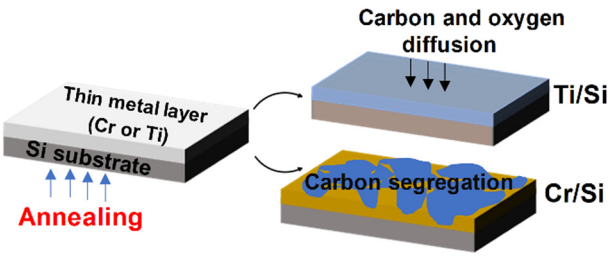
Ming-Yang Liu,* Guang-Qiang Li, Yao He and Kai Xiong



2355

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

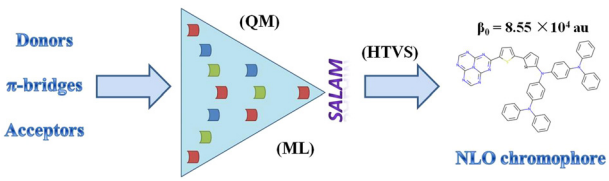
Ayesha Kousar, Ulviyya Quliyeva, Ishan Pande, Jani Sainio, Jaakko Julin, Timo Sajavaara, Antti J. Karttunen and Tomi Laurila*



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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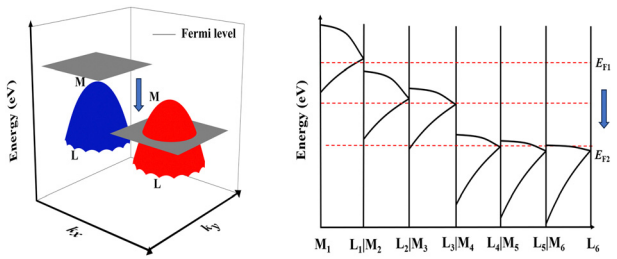
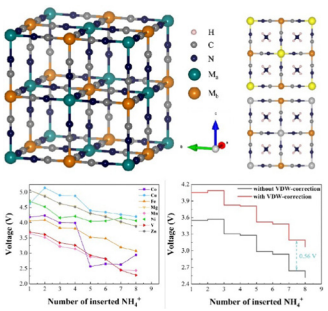


Theoretical study of CDW phases for bulk NbX_2 (X = S and Se)

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

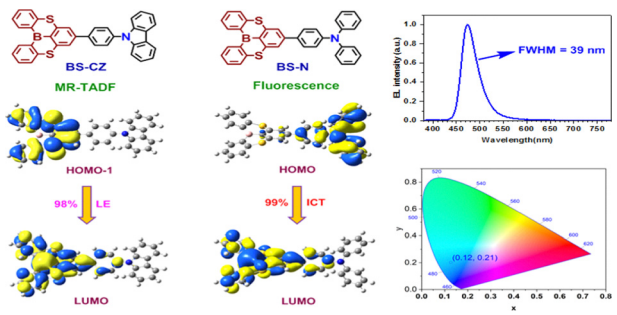
2387



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*

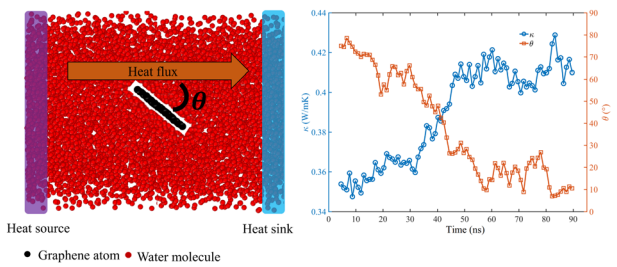
2395



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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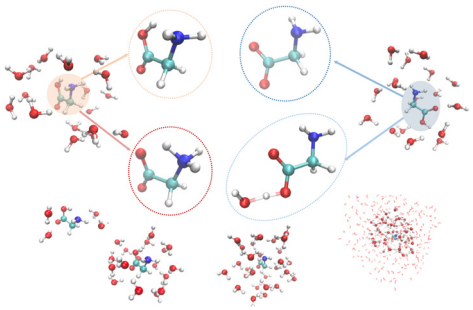
Temperature driven transformations of glycine molecules embedded in interstellar ice

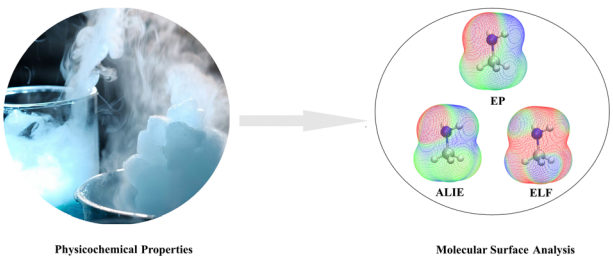
Maysa Yusef-Buey, Tzonka Mineva, Dahbia Talbi and Mathias Rapacioli*



2426

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

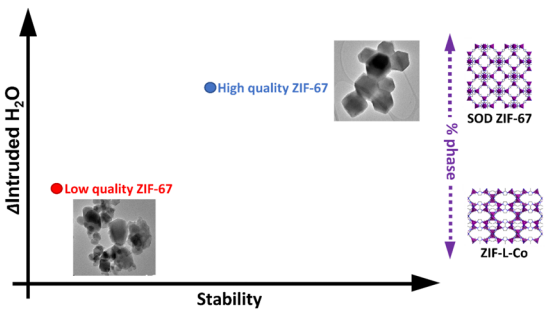
Ossama Abdeen, Mohamed Ismael* and Aly Abdou*



2440

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

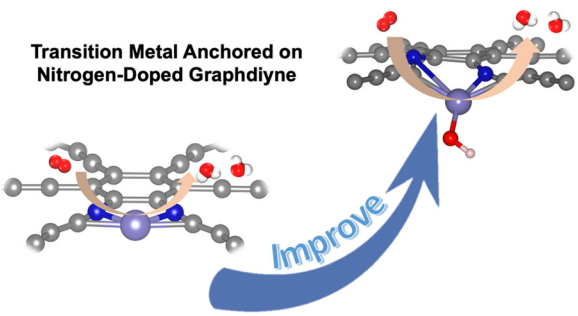
Eder Amayuelas,* Luis Bartolomé, Yan Zhang, Juan Miguel López del Amo, Oleksandr Bondarchuk, Artem Nikulin, Francisco Bonilla, Elena Palomo del Barrio, Paweł Zajdel* and Yaroslav Grosu*



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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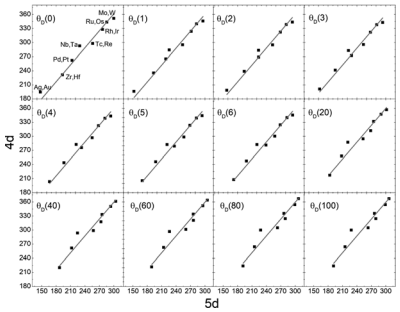
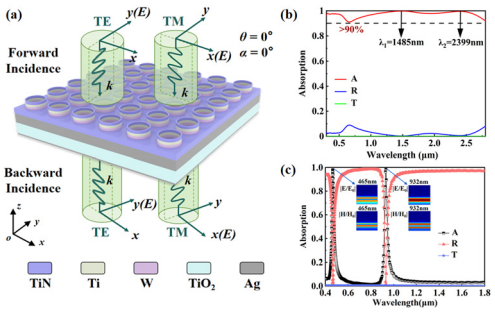


Vibrational and cohesive properties in 4d and 5d transition metals: systematics and interrelations

Dalía S. Bertoldi* and A. Fernández Guillermet

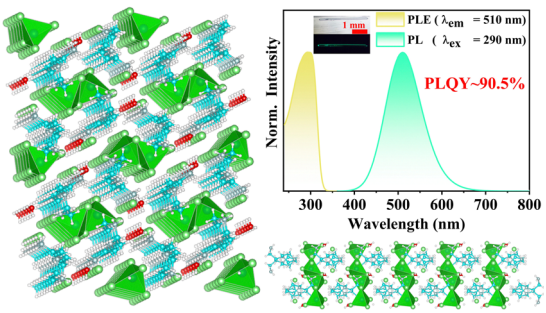
2463



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*

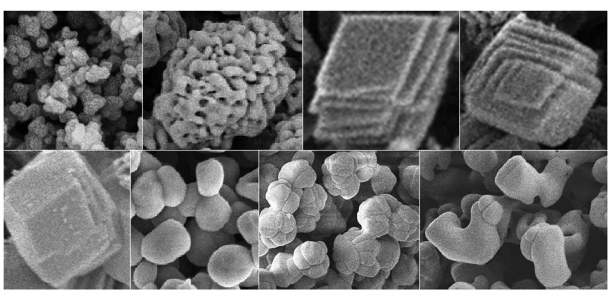
2472



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-Fe_2O_3 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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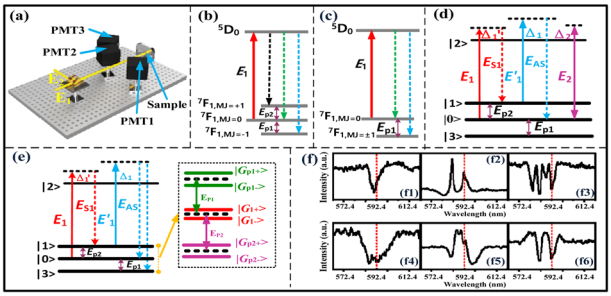
2486

Spectral and temporal atomic coherence interaction in $Eu^{3+}:NaYF_4$ and $Eu^{3+}:BiPO_4$

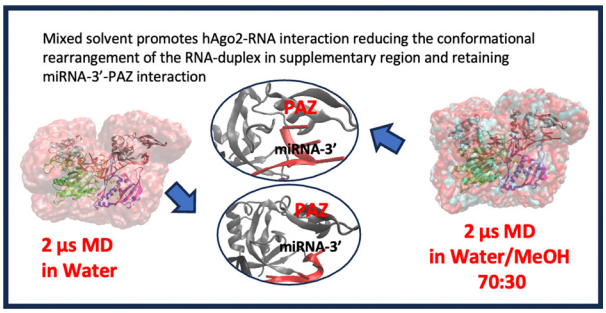
Zhou Feng, Muhammad Imran, Faisal Nadeem, Huanrong Fan, Jin Yan, Irfan Ahmed, Condon Lau* and Yanpeng Zhang*



2497

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

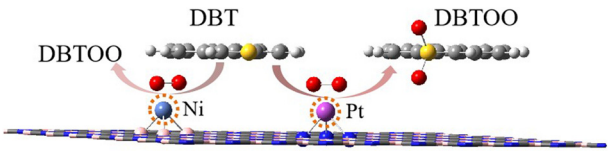
Francesco Porcelli, Anna Rita Casavola, Alessandro Grottesi, Donatella Schiumarini and Lorenzo Avaldi



2509

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

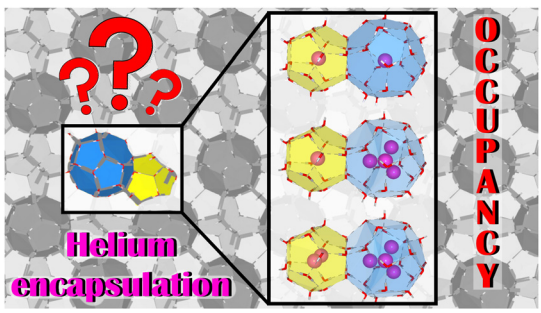
Naixia Lv, Hongshun Ran, Jinrui Zhang, Jie Yin, Yuan Zhang, Hongping Li* and Linhua Zhu*



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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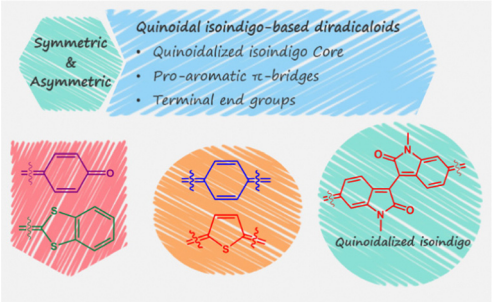
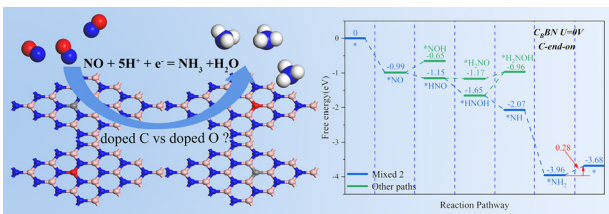


Sufficient driving force for quinoidal isoindigo-based diradicaloids with tunable diradical characters

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

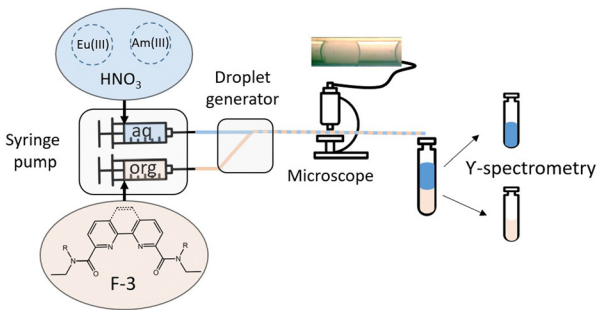
2539



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*

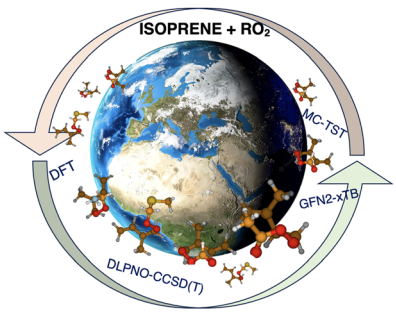
2548



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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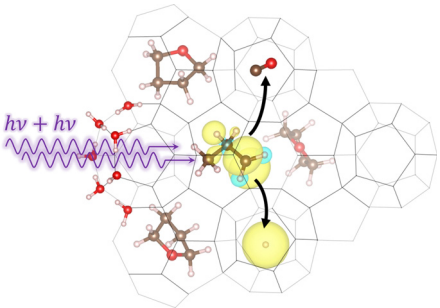
Two-photon chemistry of tetrahydrofuran in clathrate hydrates

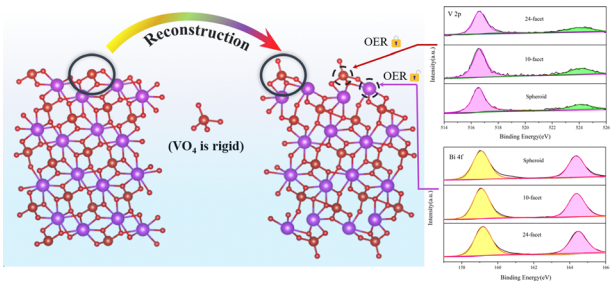
Michael A. Michon,* Pawel Chmielniak, Peter M. Weber* and Christoph Rose-Petruck*



2580

Oxygen evolution reaction (OER) active sites in $BiVO_4$ studied using density functional theory and XPS experiments

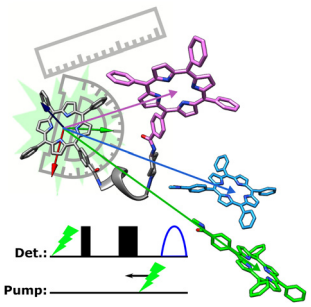
Qingyan Zhang, Guowei Liu and Taifeng Liu*



2589

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

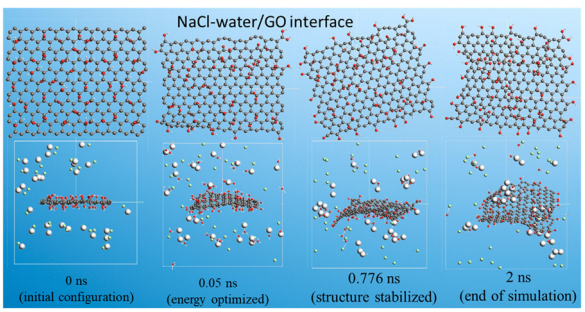
Arnau Bertran,* Marta De Zotti, Christiane R. Timmel, Marilena Di Valentin* and Alice M. Bowen*



2603

ReaxFF molecular dynamics of graphene oxide/NaCl aqueous solution interfaces

Rokhsareh Akbarzadeh and Milan Předota*



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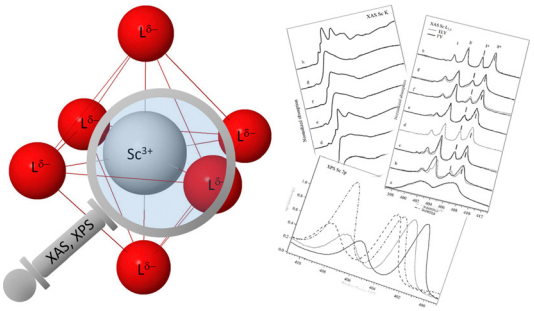
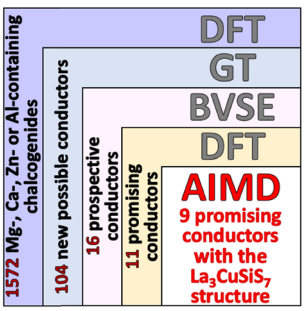


Chemical bonding effects in Sc compounds studied using X-ray absorption and X-ray photoelectron spectroscopies

Anna Zimina,* Aline Léon and Ralph Steininger

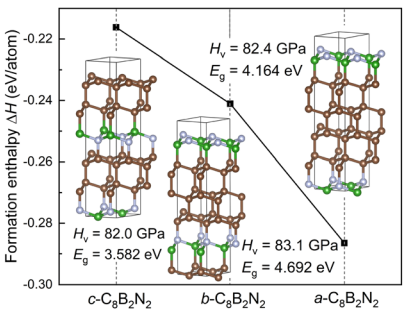
2622



A novel class of multivalent ionic conductors with the La_3CuSiS_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

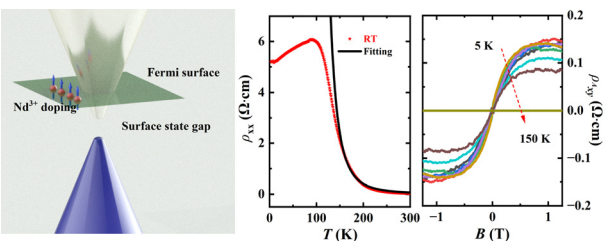
2629



Novel superhard semiconducting structures of $C_8B_2N_2$ 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 $Bi_{1.1}Sb_{0.9}STe_2$ topological insulator single crystals

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

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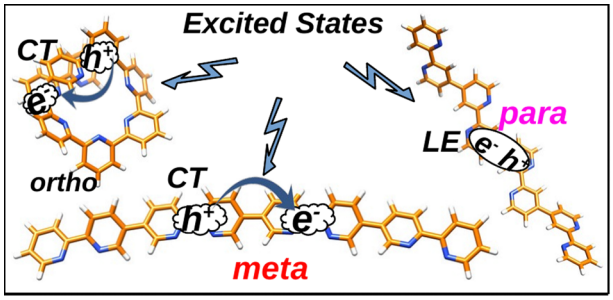
2646

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

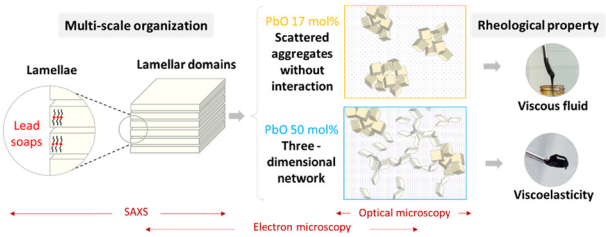
Palak Mandal and Aditya N. Panda*



2657

Multiscale organisation of lead carboxylates in artistic oil binders

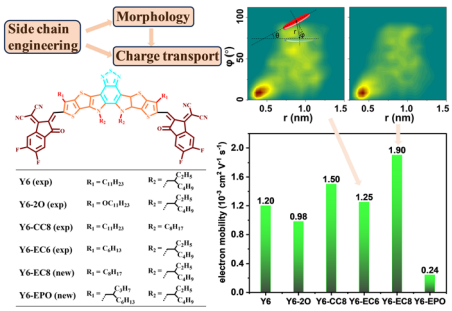
Lucie Laporte, Frédéric Gobeaux, Thierry Pouget, Nicolas Benoot, Julien Foisnon, David Touboul, Guylaine Ducouret and Laurence de Viguerie*



2666

The effects of side chain engineering on the morphology and charge transport of the A–DA$_1$D–A type of non-fullerene acceptor: a multiscale study

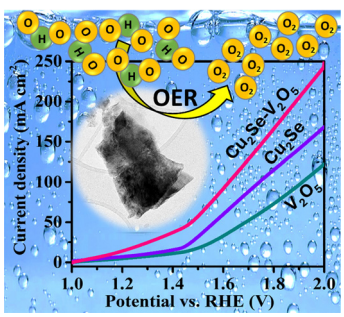
Zhijun Cao and Shaohui Zheng*



2678

Synergistic effect of a bamboo-like Bi_2S_3 covered Sm_2O_3 nanocomposite (Bi_2S_3–Sm_2O_3) 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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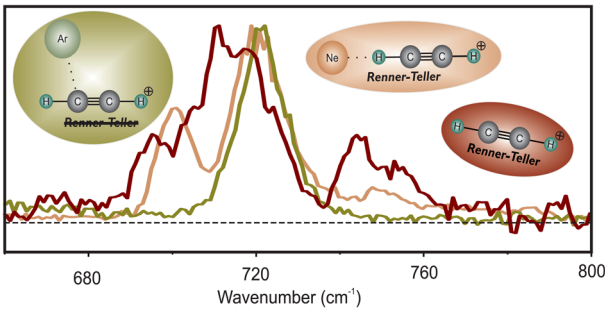

Leak-out spectroscopy as alternative method to rare-gas tagging for the Renner–Teller perturbed $HCCH^+$ and $DCCD^+$ ions

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