

IN THIS ISSUE

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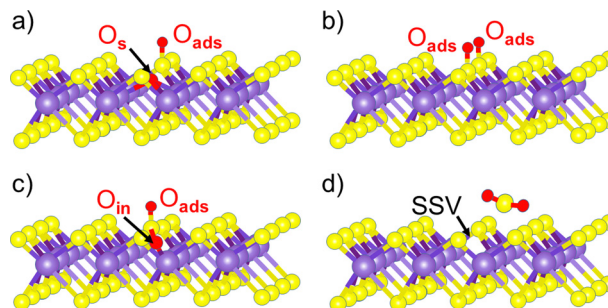
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REVIEWS

12555

A brief review on thermally induced oxidation and oxidative etching of thin MoS₂ crystals

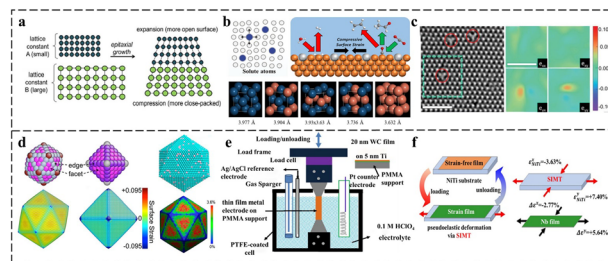
Robert Szoszkiewicz



12565

Atomic understanding of the strain-induced electrocatalysis from DFT calculation: progress and perspective

Qibo Deng, Rui Huang, Li-hua Shao,
Alexander V. Mumyatov, Pavel A. Troshin, Cuihua An,*
Shuai Wu,* Linxiao Gao, Bo Yang and Ning Hu



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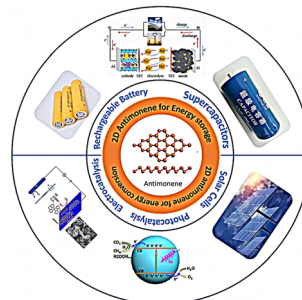


REVIEWS

12587

Research progress of two-dimensional antimonene in energy storage and conversion

Zhe Li, Yanjie Cheng, Ye Liu and Yunhui Shi*

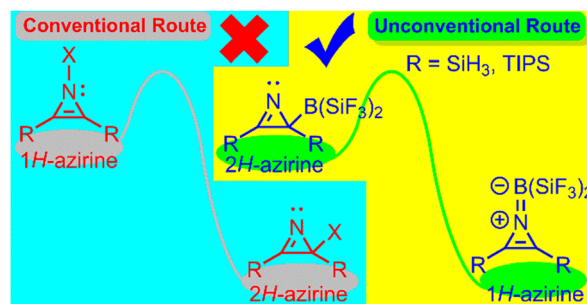


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12602

An unprecedented route to achieve persistent 1*H*-azirine

Alvi Muhammad Rouf* and Jun Zhu*

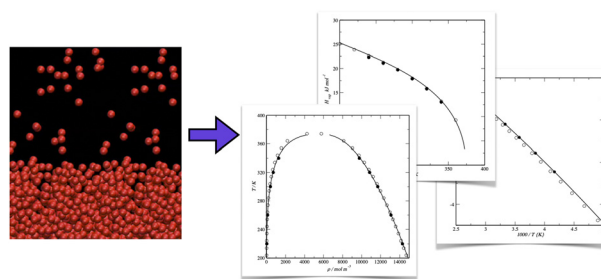


PERSPECTIVES

12607

Molecular modelling of the thermophysical properties of fluids: expectations, limitations, gaps and opportunities

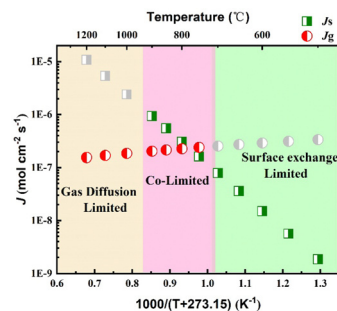
Marcus J. Tillotson, Nikolaos I. Diamantonis, Corneliu Buda, Leslie W. Bolton and Erich A. Müller*



12629

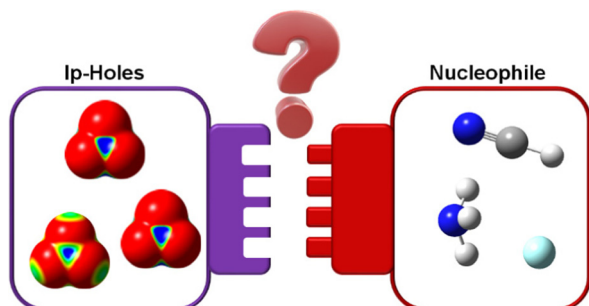
Perspective on high-temperature surface oxygen exchange in a porous mixed ionic-electronic conductor for solid oxide cells

Hairui Han, Yunan Jiang,* Shaowei Zhang and Changrong Xia*



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12641

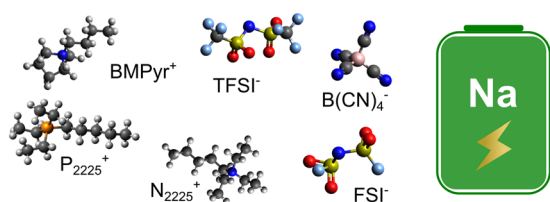


Yet another perspective on hole interactions, part II: lp-hole vs. lp-hole interactions

Rahul Shukla,* Dongkun Yu, Tiancheng Mu and Sebastian Kozuch

12650

Ionic Liquids for improved thermal stability of batteries

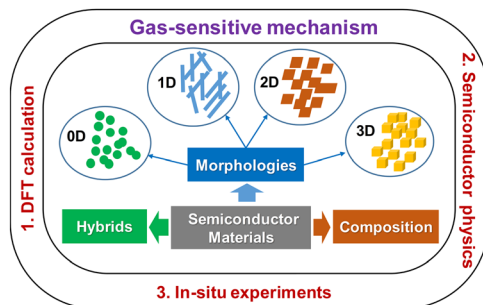


Effect of ions structures in transport properties and impact on battery performance

Ionic liquids as potential electrolytes for sodium-ion batteries: an overview

Leandro S. Domingues, Hercilio G. de Melo and Vitor L. Martins*

12668

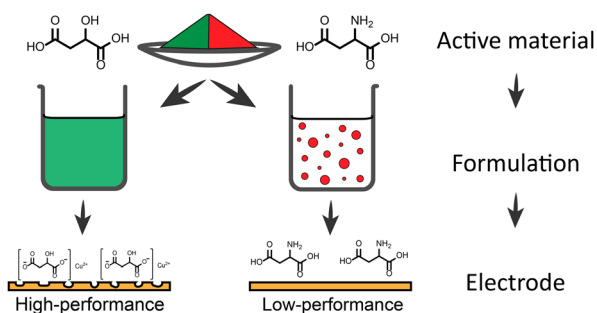


Research progress and prospects on gas-sensitive mechanisms of semiconductor sensors

Jifeng Chu, Jianbin Pan, Qiongyuan Wang, Aijun Yang,* Shizhen Song, Huan Yuan, Mingzhe Rong and Xiaohua Wang

RESEARCH PAPERS

12684



In situ synthesis of Cu(II) dicarboxylate metal organic frameworks (MOFs) and their application as battery materials

Matthew Teusner, Jitendra Mata and Neeraj Sharma*

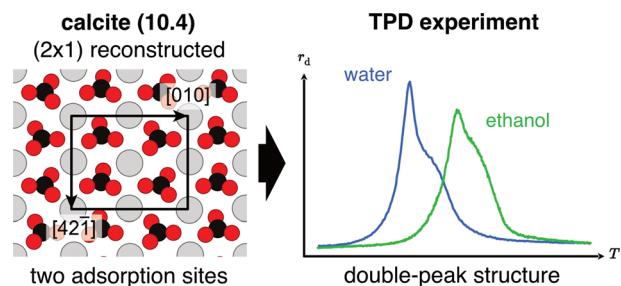


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How water desorbs from calcite

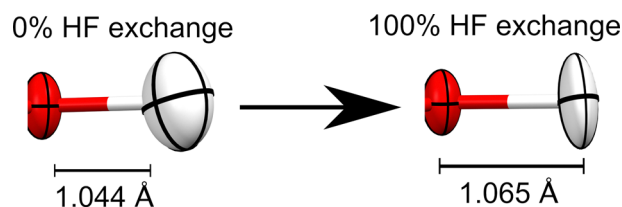
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12702

How do density functionals affect the Hirshfeld atom refinement?

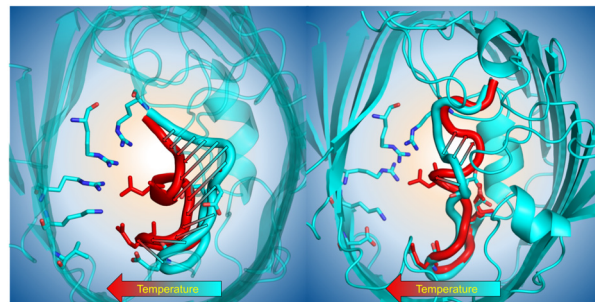
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12712

How the physical properties of bacterial porins match environmental conditions

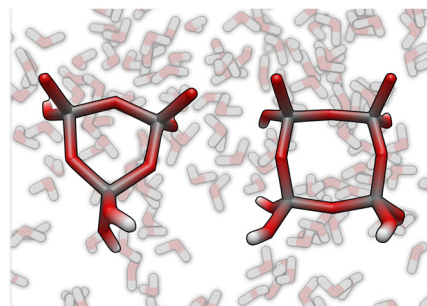
Stefan Milenkovic, Jiajun Wang, Silvia Acosta-Gutierrez,
Mathias Winterhalter, Matteo Ceccarelli* and
Igor V. Bodrenko*



12723

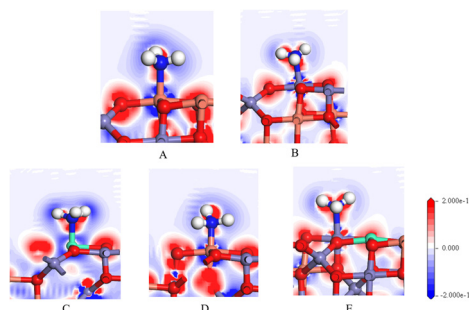
Insight into the role of excess hydroxide ions in silicate condensation reactions

Tuong Ha Do, Hien Duy Tong, Khanh-Quang Tran,
Evert Jan Meijer* and Thuat T. Trinh*



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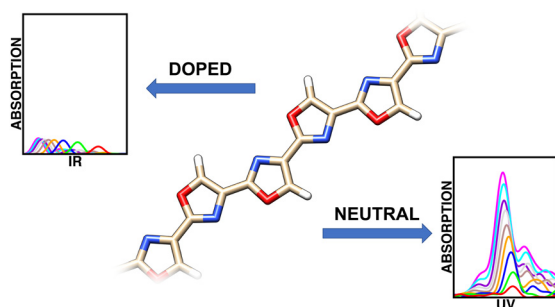
12734



Study on the mechanism of NO_x reduction by NH₃-SCR over a Zn_xCu_{1-x}Fe₂O₄ catalyst

Taoyuan Ouyang, Yaoning Bai, Xu Wang, Xinru Li, Yuwei Yan, Zichen Wang, Xiaodi Jiang, Xiaoming Cai, Jinming Cai and Honglin Tan*

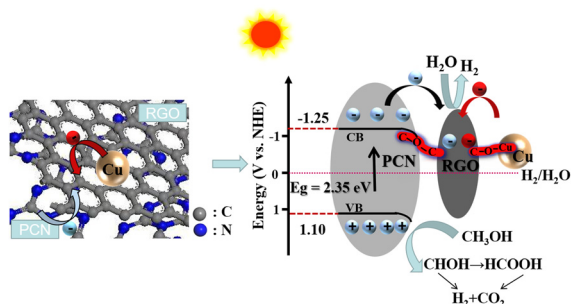
12744



First-principles study of electronic and optical properties in 1-dimensional oligomeric derivatives of telomestatin

Joëlle Mergola-Greef and Bruce F. Milne*

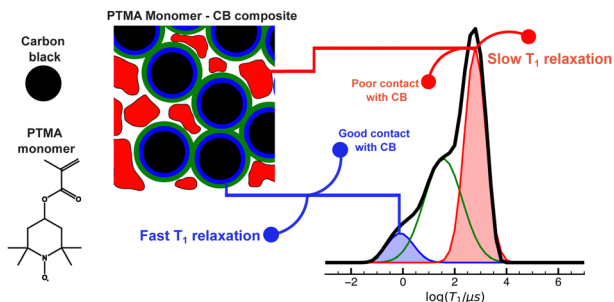
12754



Enhanced plasmonic photocatalytic performance of C₃N₄/Cu by the introduction of a reduced graphene oxide interlayer

Qixiao Gai, Shoutian Ren,* Xiaochun Zheng and Wenjun Liu*

12767



Laplace inverted pulsed EPR relaxation to study contact between active material and carbon black in Li-organic battery cathodes

Davis Thomas Daniel,* Conrad Szczuka, Peter Jakes, Rüdiger-A. Eichel and Josef Granwehr

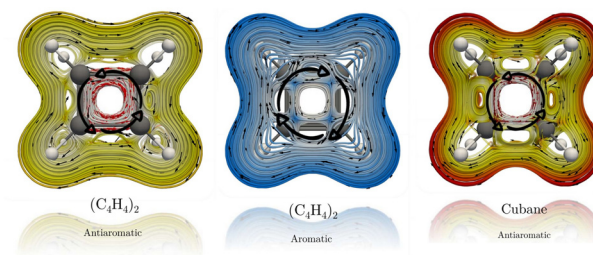


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12777

On the antiaromatic–aromatic–antiaromatic transition of the stacked cyclobutadiene dimer

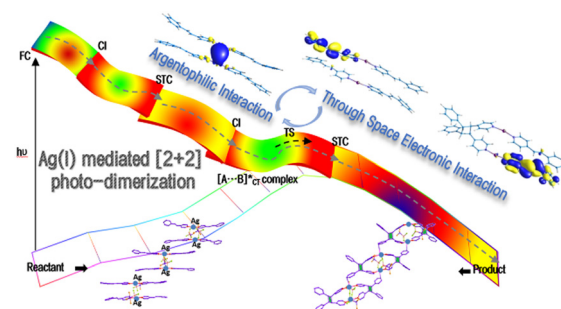
Mesías Orozco-Ic* and Dage Sundholm*



12783

Synergetic argentophilic and through space electronic interactions in a single-crystal-to-single-crystal photocycloaddition reaction: a mechanistic study

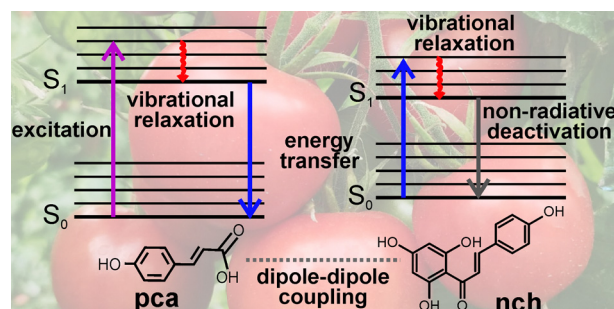
Wenjing Yang, Yonglin Chen, Min Mei, Weijia Li, Chu Wang, Yanting Yang, Jing Liang, Zhen Guo,* Liangliang Wu* and Xuebo Chen*



12791

Synergic photoprotection of phenolic compounds present in tomato fruit cuticle: a spectroscopic investigation in solution

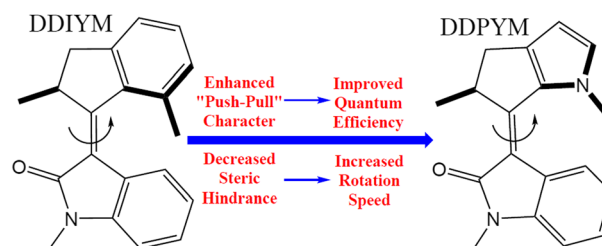
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12800

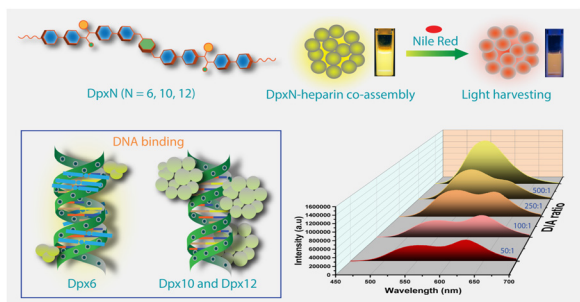
Simultaneously improving the efficiencies of photo- and thermal isomerization of an oxindole-based light-driven molecular rotary motor by a structural redesign

Jianzheng Ma, Di Zhao, Le Yu, Chenwei Jiang,* Zhenggang Lan* and Fuli Li



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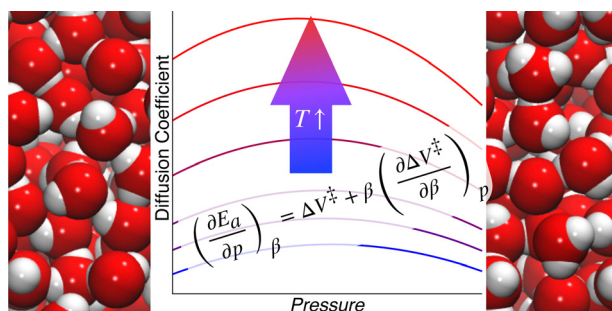
12810



Contrasting luminescence in heparin and DNA-templated co-assemblies of dimeric cyanostilbenes: efficient energy transfer in heparin-based co-assemblies

Dhananjoy Maity, Shubhra Kanti Bhaumik and Supratim Banerjee*

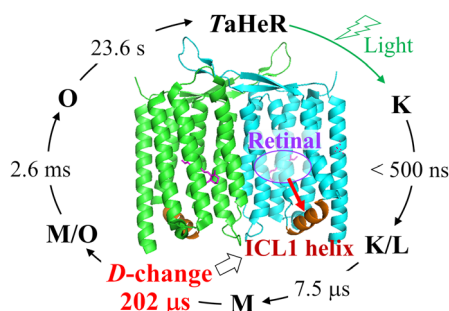
12820



A Maxwell relation for dynamical timescales with application to the pressure and temperature dependence of water self-diffusion and shear viscosity

Zeke A. Piskulich, Ashley K. Borkowski and Ward H. Thompson*

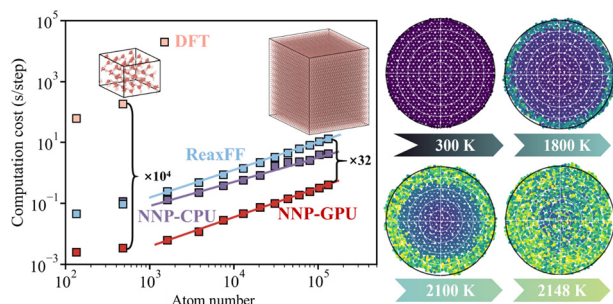
12833



Time-resolved detection of light-induced conformational changes of heliorhodopsin

Yusuke Nakasone, Yuma Kawasaki, Masae Konno, Keiichi Inoue and Masahide Terazima*

12841



Monitoring the melting behavior of boron nanoparticles using a neural network potential

Xiaoya Chang, Qingzhao Chu and Dongping Chen*

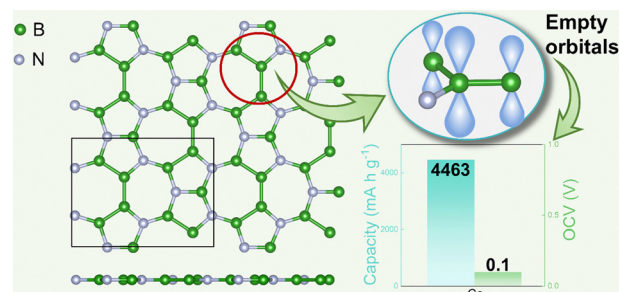


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12854

B₅N₃ as a potential high-capacity electrode material for calcium ion batteries

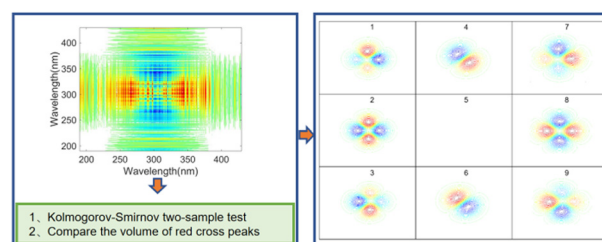
Yu Xiong, Ninggui Ma, Yuhang Wang, Tairan Wang, Shuang Luo and Jun Fan*



12863

A new approach to recognizing the correct pattern of cross-peaks from a noisy 2D asynchronous spectrum by detecting intrinsic symmetry via the Kolmogorov–Smirnov test

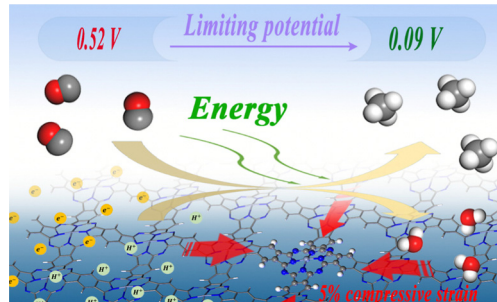
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12872

Unexpected electro-catalytic activity of the CO reduction reaction on Cr-embedded poly-phthalocyanine realized by strain engineering: a computational study

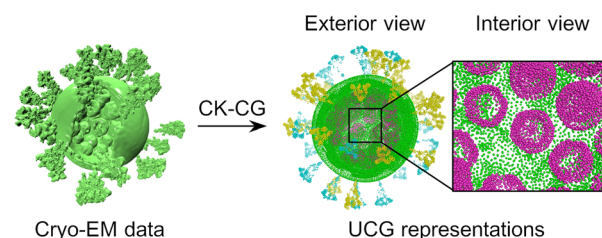
Wenzhen Xu, Yunpeng Shu, Mengmeng Xu, Juan Xie, Youyong Li* and Huilong Dong*



12882

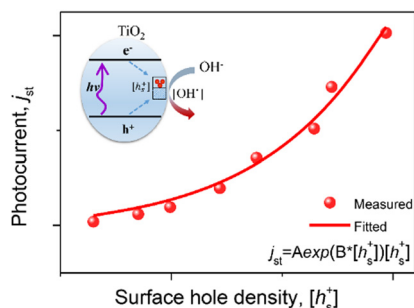
Development of multiscale ultra-coarse-grained models for the SARS-CoV-2 virion from cryo-electron microscopy data

Fengyu Li, Yuwei Zhang, Fei Xia* and Xin Xu*



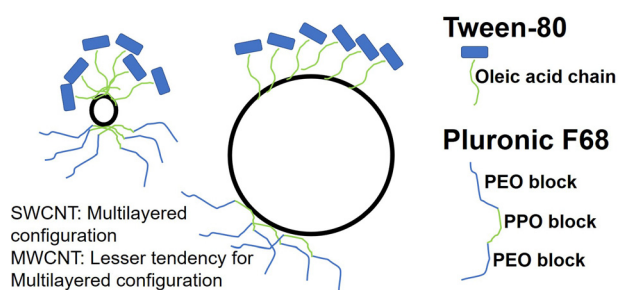
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12891

Unconventional rate law of water photooxidation at TiO_2 electrodes

Shufeng Zhang,* Wenhua Leng and Kai Liu*

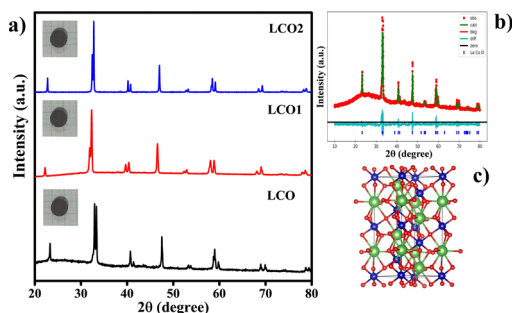
12900



HRMAS-NMR and simulation study of the self-assembly of surfactants on carbon nanotubes

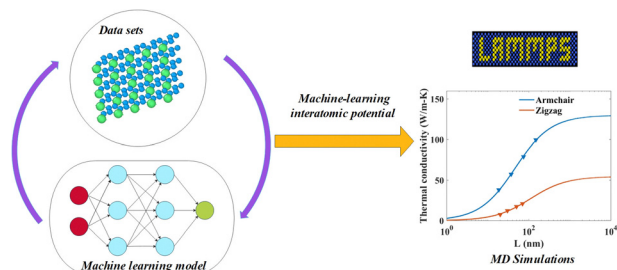
Raman Preet Singh* and Taranpreet Kaur

12914

Small polaron hopping conduction mechanism and enhanced thermoelectric power factor in the perovskite LaCoO_3 ceramic

K. P. Mohamed Jibri, J. Archana, M. Navaneethan* and S. Harish*

12923

Lattice thermal conductivity and Young's modulus of XN_4 (X = Be, Mg and Pt) 2D materials using machine learning interatomic potentials

Khashayar Ghorbani, Pedram Mirchi, Saeed Arabha, Ali Rajabpour* and Sebastian Volz*

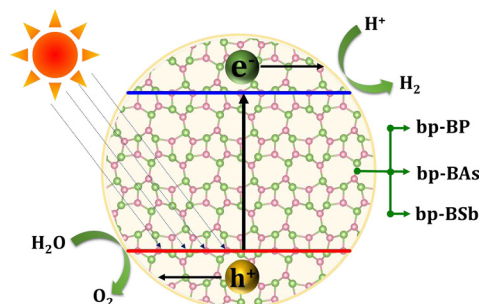


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12934

Boron–pnictogen monolayers with a negative Poisson's ratio and excellent band edge positions for photocatalytic water splitting

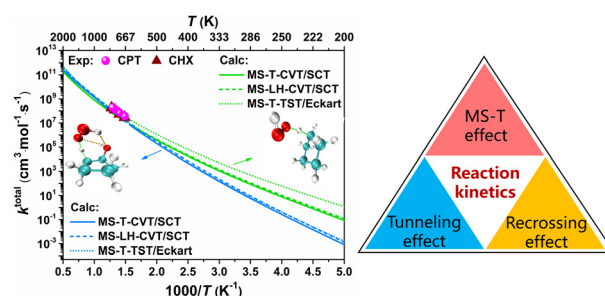
Naga Venkateswara Rao Nulakani and T. J. Dhillip Kumar*



12943

Multi-structural variational kinetics study on hydrogen abstraction reactions of cyclopentanol and cyclopentane by hydroperoxyl radical with anharmonicity, recrossing and tunneling effects

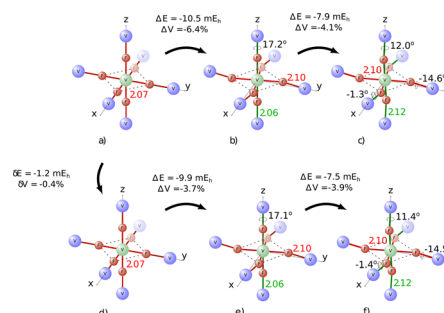
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12961

The role of the A monovalent cation in the AVF₃ perovskite series. A quantum mechanical investigation

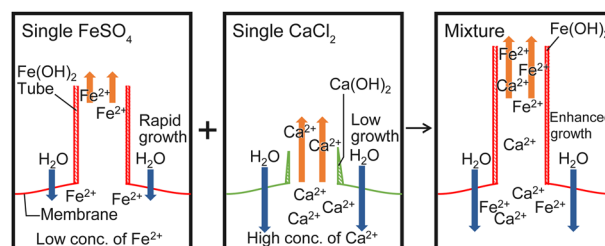
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12974

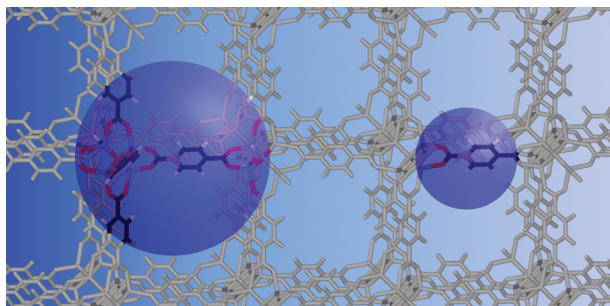
Characteristic growth of chemical gardens from mixtures of two salts

Yujin Kubodera, Yu Xu, Yuta Yamaguchi, Muneyuki Matsuo, Masashi Fujii, Maya Kageyama, Oliver Steinbock and Satoshi Nakata*



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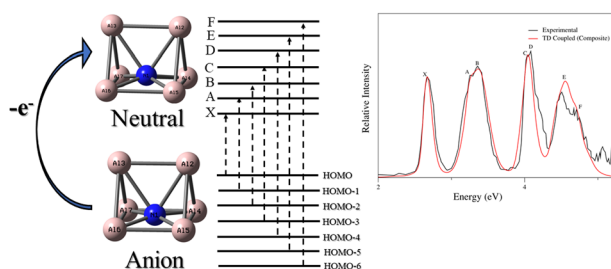
12979



Machine learning transferable atomic forces for large systems from underconverged molecular fragments

Marius Herbold and Jörg Behler*

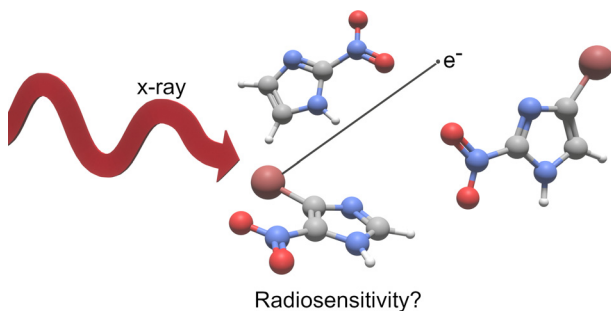
12990



A theoretical study of vibronic coupling in the photoelectron spectra of Al_6N^-

Rishabh Kumar Pandey, Korutla Srikanth, Anuj Tak, Abhishek Kumar and Tammineni Rajagopala Rao*

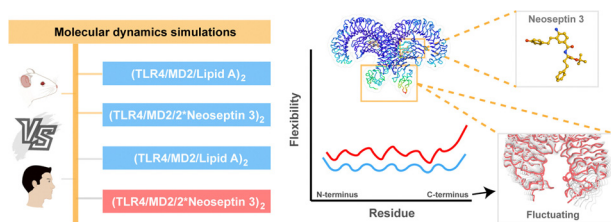
13004



Photodissociation of bromine-substituted nitroimidazole radiosensitizers

Lassi Pihlava,* Marta Berholts, Johannes Niskanen, Anton Vladyka, Kuno Kooser, Christian Strählmán, Per Eng-Johnsson, Antti Kivimäki and Edwin Kukk

13012



Dissecting the species-specific recognition of Neoseptin 3 by TLR4/MD2 via molecular dynamics simulations

Siru Wu, Cong Zhang, Yibo Wang, Penghui Li, Xiubo Du and Xiaohui Wang*

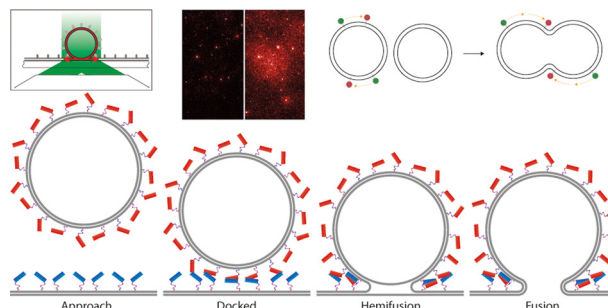


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13019

SNARE mimic peptide triggered membrane fusion kinetics revealed using single particle techniques

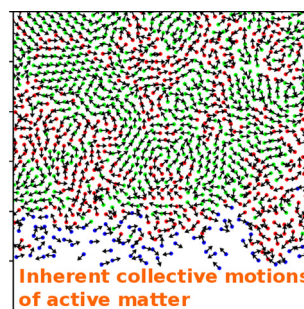
Guus van der Borg, Niek Crone, Aimee L. Boyle, Alexander Kros and Wouter H. Roos*



13027

The coherent motions of thermal active Brownian particles

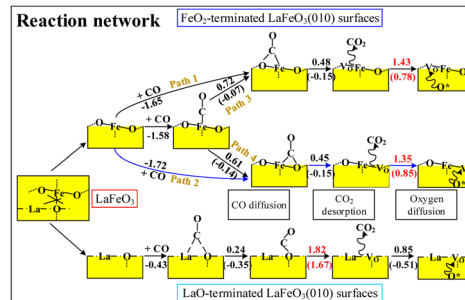
Cheng Yang, Ying Zeng, Shun Xu* and Xin Zhou*



13033

Exploration of the reaction mechanism of the LaFeO₃ oxygen carrier for chemical-looping steam methane reforming: a DFT study

Yuchuan Feng, Xiude Hu, Xin Guo and Nana Wang*



13041

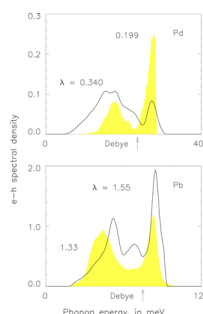
Coverage-dependent adsorption and dissociation of H₂O on Al surfaces

Pengqi Hai, Chao Wu,* Xiangdong Ding* and Yuanjie Li*



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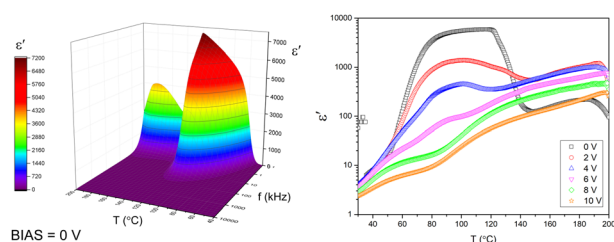
13049



On the use of Monkhorst–Pack scheme to evaluate superconductivity and the issue of umklapp electron–phonon interactions

X. H. Zheng* and J. X. Zheng

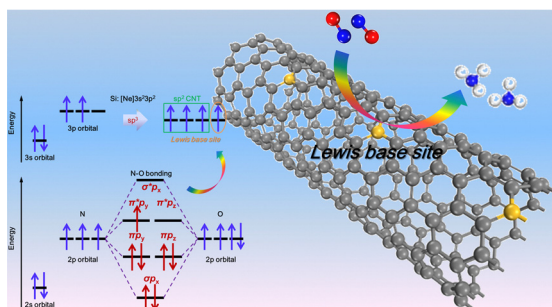
13061



Ferroelectricity in a nematic liquid crystal under a direct current electric field

Mateusz Mrukiewicz,* Paweł Perkowski, Jakub Karcz and Przemysław Kula

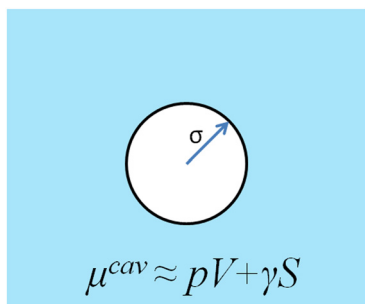
13072



Single silicon-doped CNT as a metal-free electrode for robust nitric oxide reduction utilizing a Lewis base site: an ingenious electronic “Reflux-Feedback” mechanism

Lei Yang, Jiake Fan and Weihua Zhu*

13080



A cavity formation energy formula for hard spheres in simple electrolyte solutions

Tiejun Xiao* and Yun Zhou

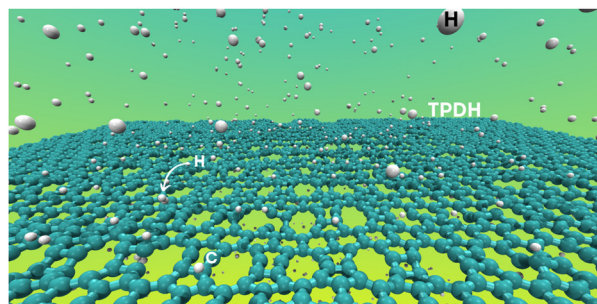


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13088

Tetra-penta-deca-hexagonal-graphene (TPDH-graphene) hydrogenation patterns: dynamics and electronic structure

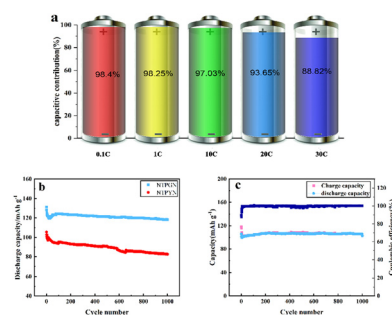
Caique C. Oliveira, Matheus Medina, Douglas S. Galvao and Pedro A. S. Autreto*



13094

N-modified carbon-coated $\text{NaTi}_2(\text{PO}_4)_3$ as an anode with high capacity and long lifetime for sodium-ion batteries

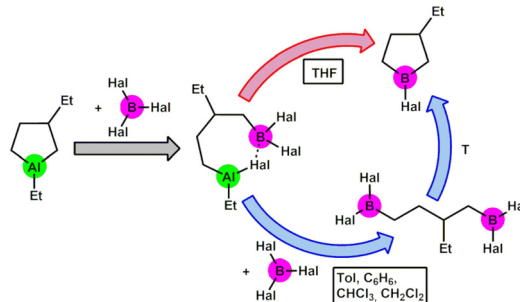
Shuang Ding, Huijin Li, Jie Yuan,* Xianli Yuan and Min Li



13104

The mechanism of the replacement of aluminum atoms in 1-ethyl-3-alkylalumolanes by boron atoms with boron halides

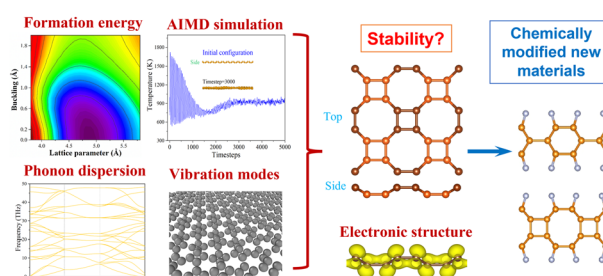
T. V. Tyumkina,* L. I. Tulyabaeva, S. M. Idrisova, D. N. Islamov, L. M. Khalilov and U. M. Dzhemilev



13116

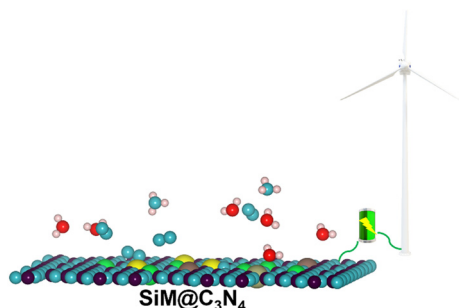
Theoretical insights into the stability of buckled tetragonal graphene and the prediction of novel carbon allotropes

Chao Cheng, Xin Zhang, Shangyi Ma* and Shaoqing Wang



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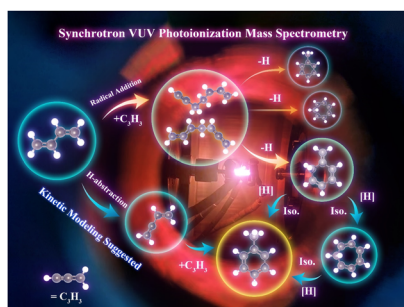
13126



Efficient asymmetrical silicon–metal dimer electrocatalysts for the nitrogen reduction reaction

Chuangwei Liu, Haoren Zheng, Tianyi Wang, Xiaoli Zhang, Zhongyuan Guo* and Hao Li*

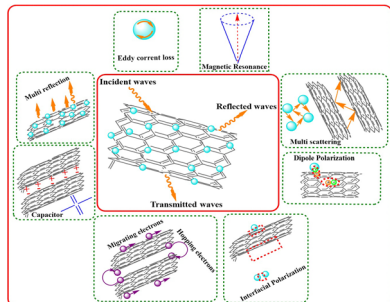
13136



Elucidating the toluene formation mechanism in the reaction of propargyl radical with 1,3-butadiene

Jianhui Jin, Cheng Xie, Jiao Gao, Hong Wang, Jinyang Zhang, Yujie Zhao,* Min Gao, Jiabi Ma, Zhandong Wang and Jiwen Guan*

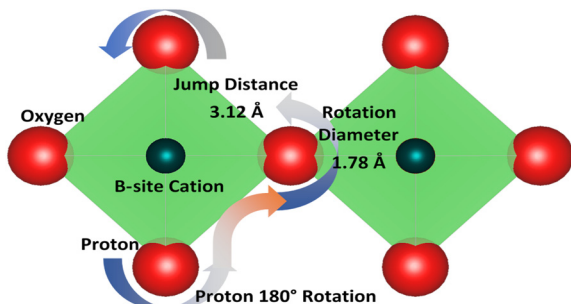
13145



Superior microwave absorption ability of CuFe₂O₄/MWCNT at whole Ku-band and half X-band

Mahla Tahamipoor and Hoda Hekmatara*

13155



Proton dynamics in a spark-plasma sintered BaZr_{0.7}Ce_{0.2}Y_{0.1}O_{3-δ} proton conductor investigated by quasi-elastic neutron scattering

J. Wallis,* A. Kruth and F. Demmel

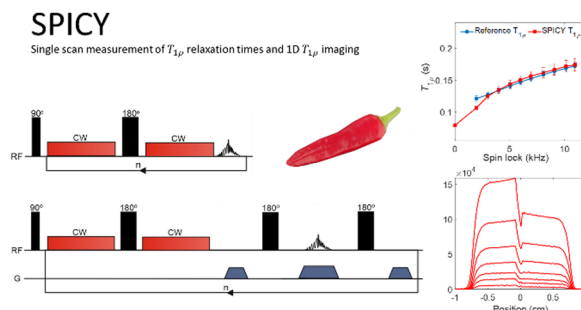


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13164

SPICY: a method for single scan rotating frame relaxometry

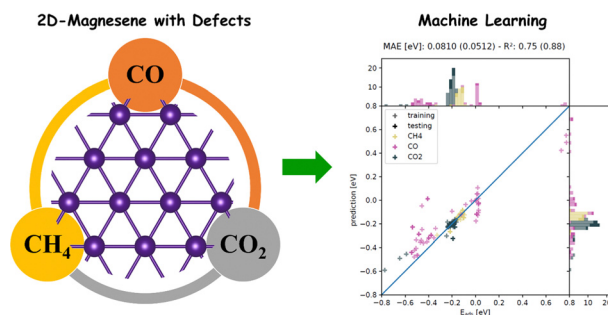
Katja Tolkkinen, Sarah E. Mailhot, Anne Selent, Otto Mankinen, Henning Henschel, Miika T. Nieminen, Matti Hanni, Anu M. Kantola, Timo Liimatainen and Ville-Veikko Telkki*



13170

Machine learning and DFT investigation of CO, CO₂ and CH₄ adsorption on pristine and defective two-dimensional magnesene

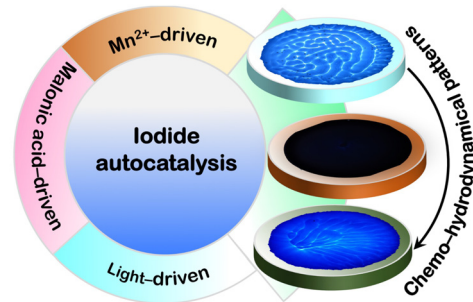
Siby Thomas,* Felix Mayr, Ajith Kulangara Madam and Alessio Gagliardi*



13183

Multiple iodide autocatalysis paths of chemo-hydrodynamical patterns in the Briggs–Rauscher reaction

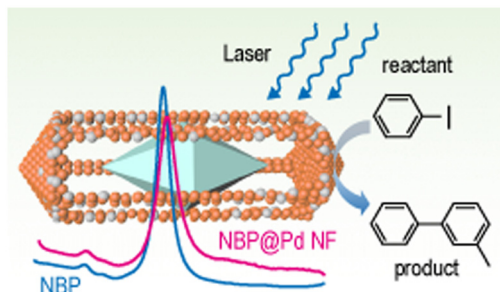
Ling Yuan,* Hongzhang Wang, Chunxiao Meng, Zhenfang Cheng, Xiaoli Lv and Qingyu Gao*



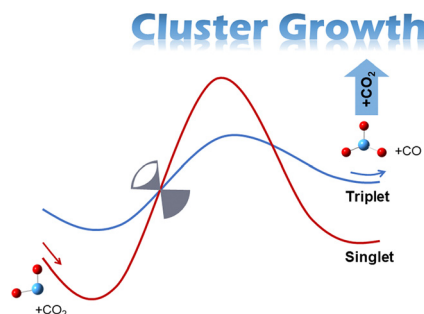
13189

Plasmonic and catalytic Au NBP@AgPd nanoframes for highly efficient photocatalytic reactions

Juan Xu, Haiying Xu, Lihui Xu, Qifeng Ruan, Xingzhong Zhu,* Caixia Kan* and Daning Shi*



13198



Infrared photodissociation spectroscopy of mass-selected $[\text{TaO}_3(\text{CO}_2)_n]^+$ ($n = 2-5$) complexes in the gas phase

Jia Han, Yang Yang, Binglin Qiu, Pengcheng Liu, Xiangkun Wu, Guanjun Wang,* Shilin Liu and Xiaoguo Zhou*

