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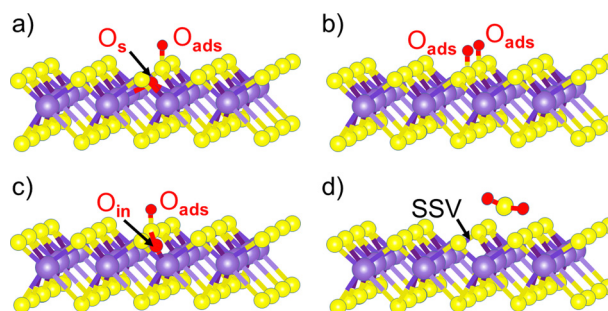
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REVIEWS

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

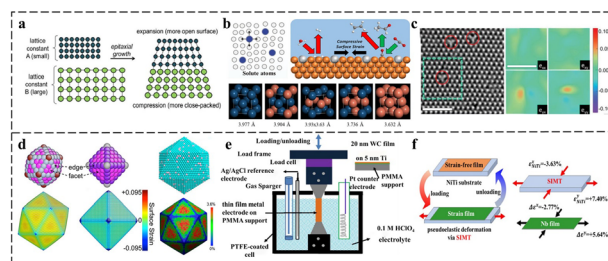
Robert Szoszkiewicz



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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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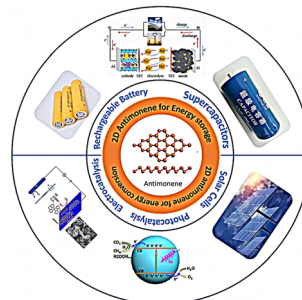


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Research progress of two-dimensional antimonene in energy storage and conversion

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

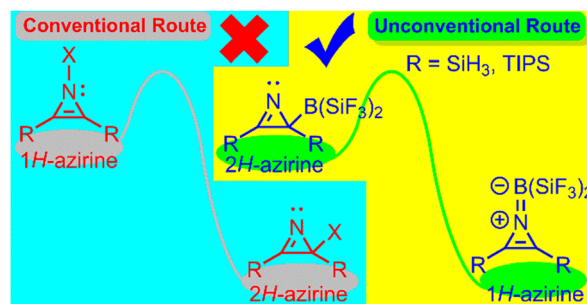


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An unprecedented route to achieve persistent 1*H*-azirine

Alvi Muhammad Rouf* and Jun Zhu*

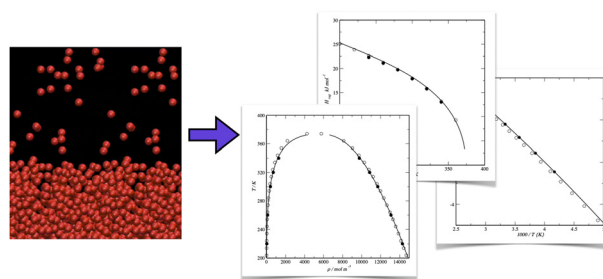


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Molecular modelling of the thermophysical properties of fluids: expectations, limitations, gaps and opportunities

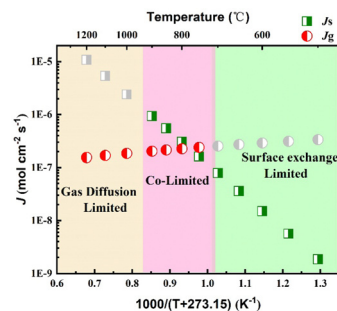
Marcus J. Tillotson, Nikolaos I. Diamantonis, Corneliu Buda, Leslie W. Bolton and Erich A. Müller*



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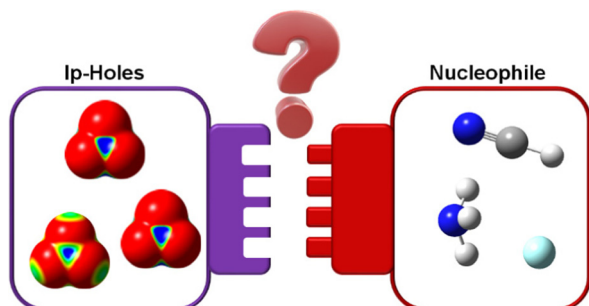
Perspective on high-temperature surface oxygen exchange in a porous mixed ionic-electronic conductor for solid oxide cells

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



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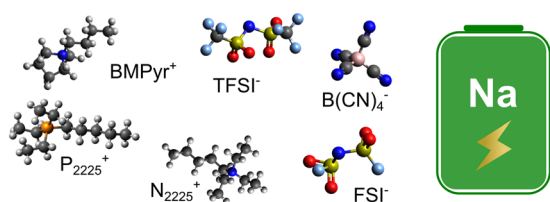


Yet another perspective on hole interactions, part II: lp-hole vs. lp-hole interactions

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

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Ionic Liquids for improved thermal stability of batteries

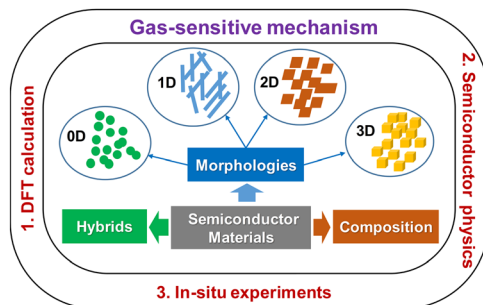


Effect of ions structures in transport properties and impact on battery performance

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

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

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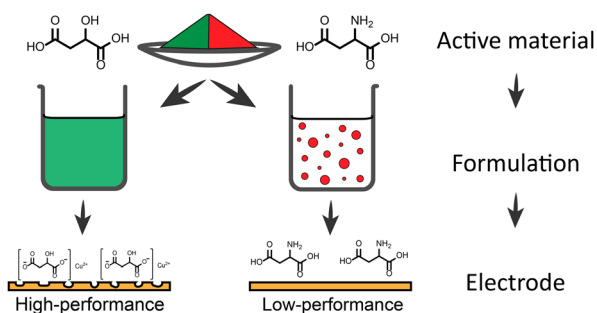


Research progress and prospects on gas-sensitive mechanisms of semiconductor sensors

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

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

Matthew Teusner, Jitendra Mata and Neeraj Sharma*

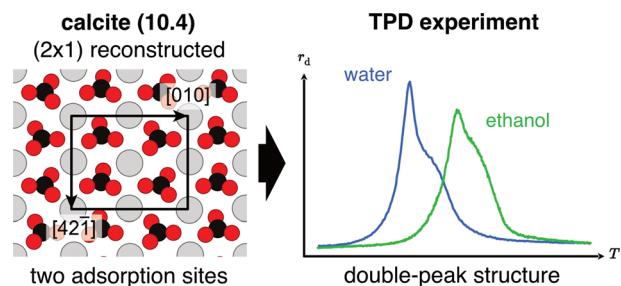


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How water desorbs from calcite

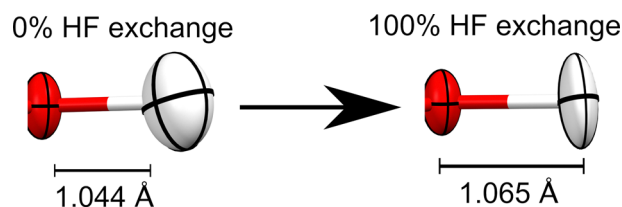
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How do density functionals affect the Hirshfeld atom refinement?

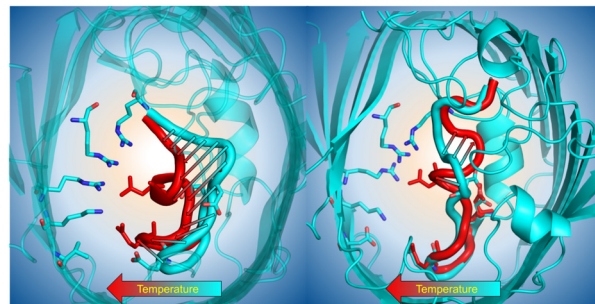
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Julia Contreras-García*



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How the physical properties of bacterial porins match environmental conditions

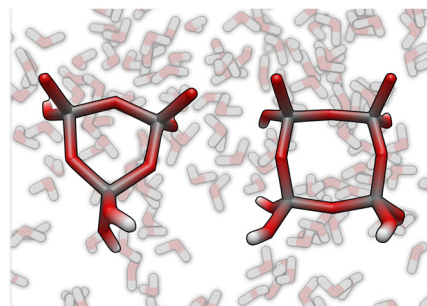
Stefan Milenkovic, Jiajun Wang, Silvia Acosta-Gutierrez,
Mathias Winterhalter, Matteo Ceccarelli* and
Igor V. Bodrenko*



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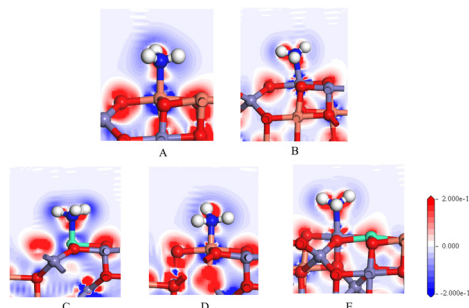
Insight into the role of excess hydroxide ions in silicate condensation reactions

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



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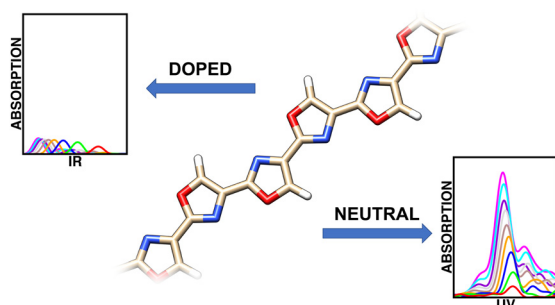
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Study on the mechanism of NO_x reduction by NH₃-SCR over a Zn_xCu_{1-x}Fe₂O₄ catalyst

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

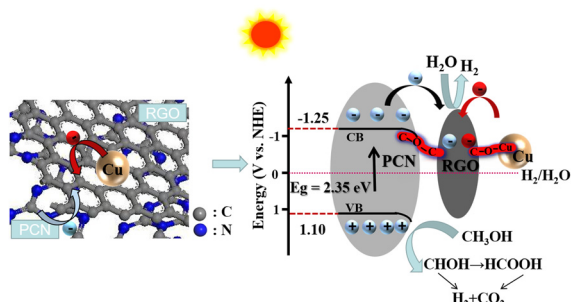
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First-principles study of electronic and optical properties in 1-dimensional oligomeric derivatives of telomestatin

Joëlle Mergola-Greef and Bruce F. Milne*

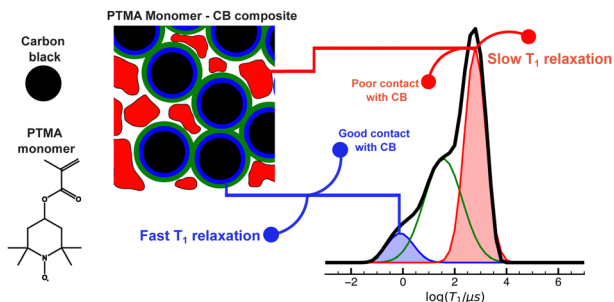
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Enhanced plasmonic photocatalytic performance of C₃N₄/Cu by the introduction of a reduced graphene oxide interlayer

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

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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

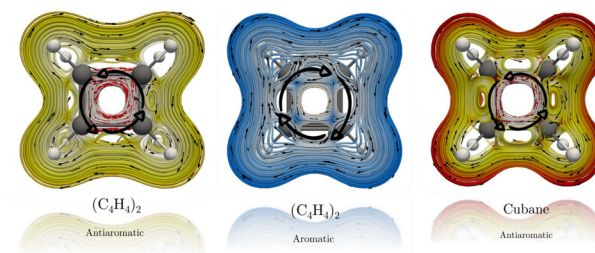


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On the antiaromatic–aromatic–antiaromatic transition of the stacked cyclobutadiene dimer

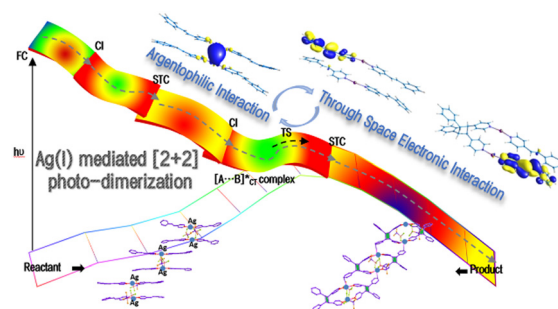
Mesías Orozco-Ic* and Dage Sundholm*



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

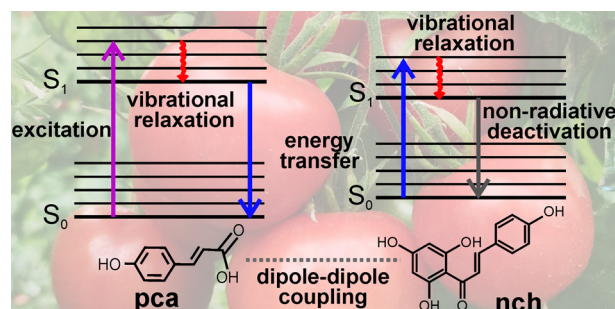
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Synergic photoprotection of phenolic compounds present in tomato fruit cuticle: a spectroscopic investigation in solution

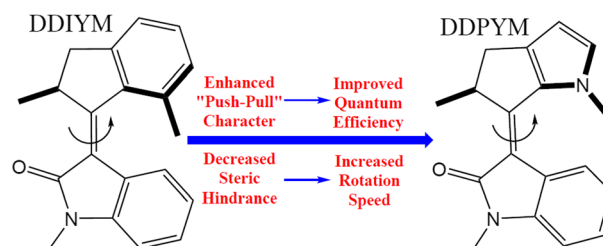
Ana González Moreno,* Jack M. Woolley, Eva Domínguez, Abel de Cózar, Antonio Heredia and Vasilios G. Stavros*



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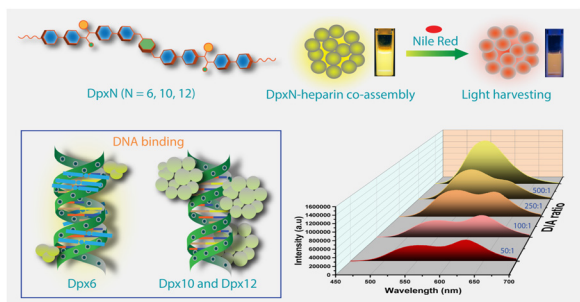
Simultaneously improving the efficiencies of photo- and thermal isomerization of an oxindole-based light-driven molecular rotary motor by a structural redesign

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



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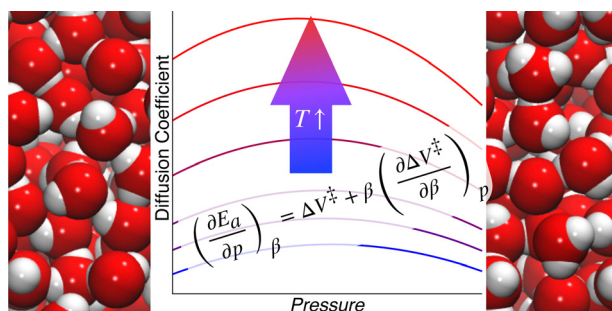
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Contrasting luminescence in heparin and DNA-templated co-assemblies of dimeric cyanostilbenes: efficient energy transfer in heparin-based co-assemblies

Dhananjoy Maity, Shubhra Kanti Bhaumik and Supratim Banerjee*

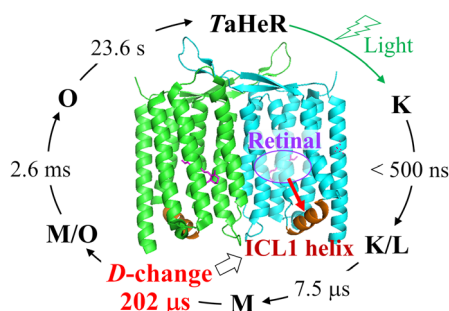
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A Maxwell relation for dynamical timescales with application to the pressure and temperature dependence of water self-diffusion and shear viscosity

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

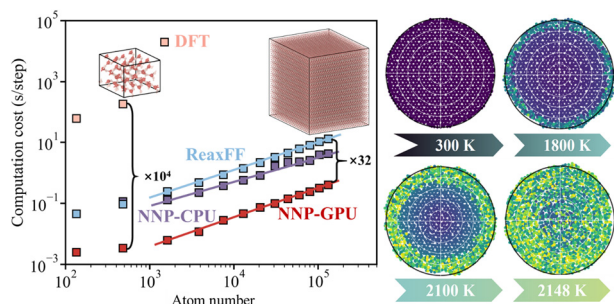
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Time-resolved detection of light-induced conformational changes of heliorhodopsin

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

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

Xiaoya Chang, Qingzhao Chu and Dongping Chen*

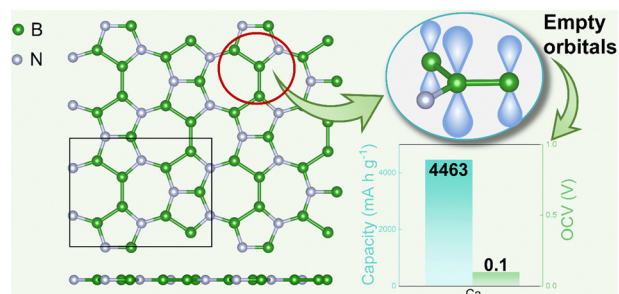


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B₅N₃ as a potential high-capacity electrode material for calcium ion batteries

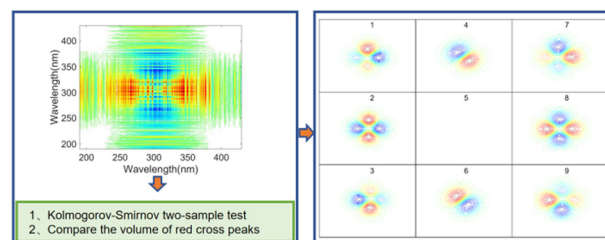
Yu Xiong, Ninggui Ma, Yuhang Wang, Tairan Wang, Shuang Luo and Jun Fan*



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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

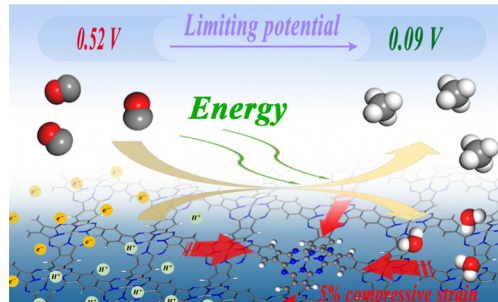
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Unexpected electro-catalytic activity of the CO reduction reaction on Cr-embedded poly-phthalocyanine realized by strain engineering: a computational study

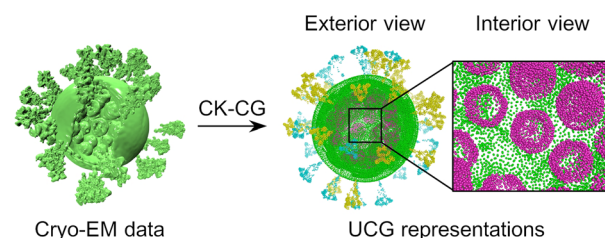
Wenzhen Xu, Yunpeng Shu, Mengmeng Xu, Juan Xie, Youyong Li* and Huilong Dong*



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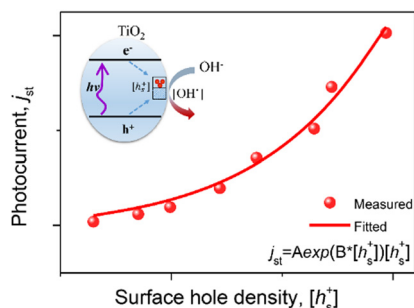
Development of multiscale ultra-coarse-grained models for the SARS-CoV-2 virion from cryo-electron microscopy data

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



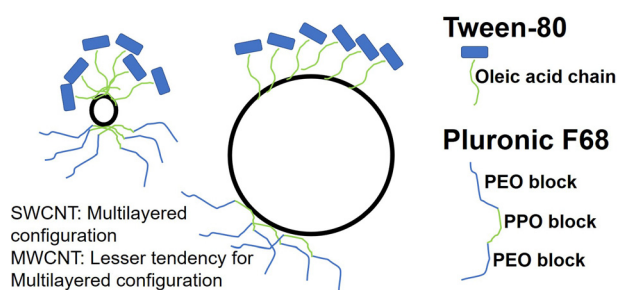
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Unconventional rate law of water photooxidation at TiO₂ electrodes

Shufeng Zhang,* Wenhua Leng and Kai Liu*

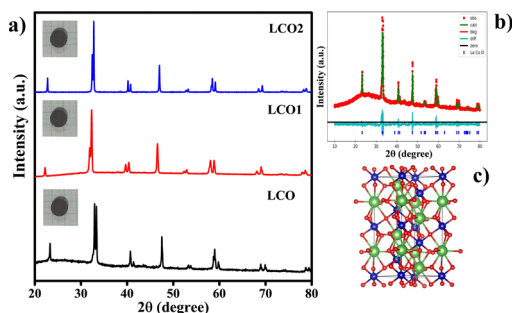
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HRMAS-NMR and simulation study of the self-assembly of surfactants on carbon nanotubes

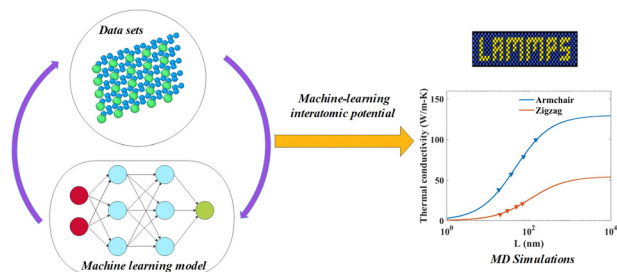
Raman Preet Singh* and Taranpreet Kaur

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Small polaron hopping conduction mechanism and enhanced thermoelectric power factor in the perovskite LaCoO₃ ceramic

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

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Lattice thermal conductivity and Young's modulus of XN₄ (X = Be, Mg and Pt) 2D materials using machine learning interatomic potentials

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

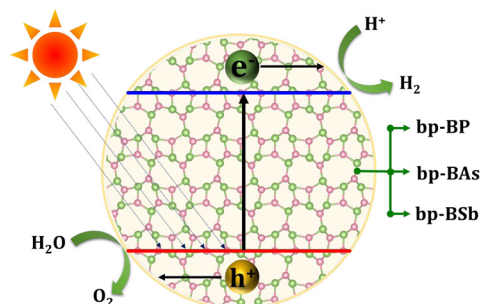


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Boron–pnictogen monolayers with a negative Poisson's ratio and excellent band edge positions for photocatalytic water splitting

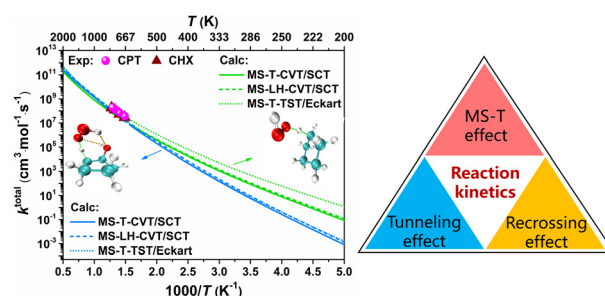
Naga Venkateswara Rao Nulakani and T. J. Dhillip Kumar*



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

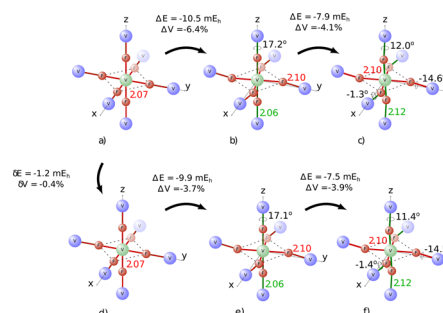
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The role of the A monovalent cation in the AVF₃ perovskite series. A quantum mechanical investigation

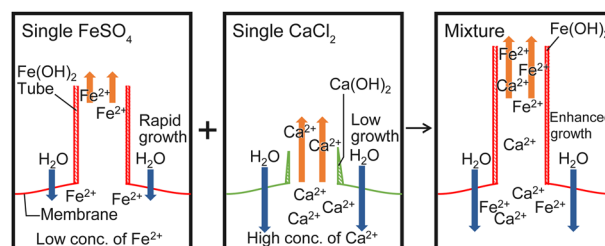
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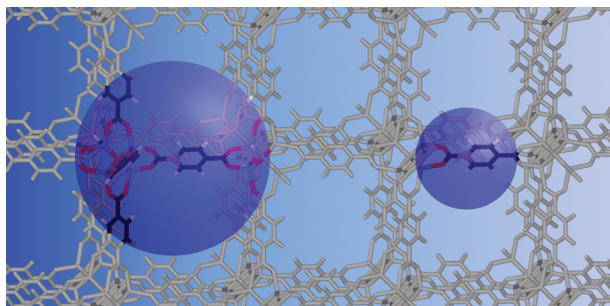
Characteristic growth of chemical gardens from mixtures of two salts

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



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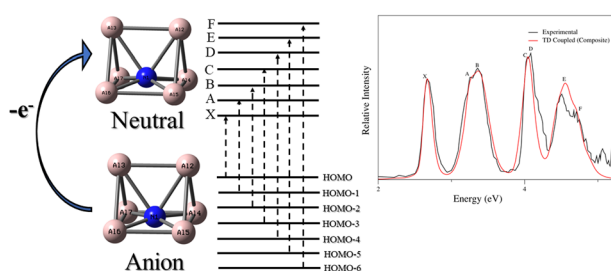
12979



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

Marius Herbold and Jörg Behler*

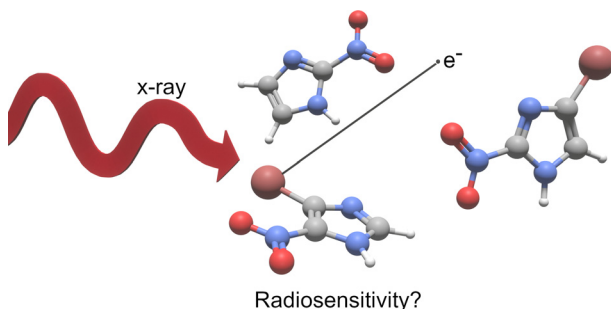
12990



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*

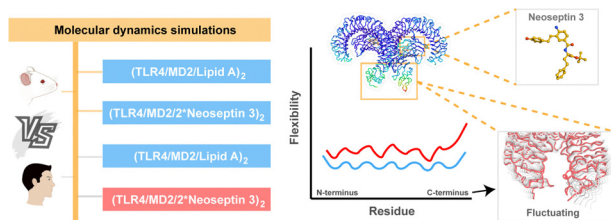
13004



Photodissociation of bromine-substituted nitroimidazole radiosensitizers

Lassi Pihlava,* Marta Berholts, Johannes Niskanen, Anton Vladyka, Kuno Kooser, Christian Strählmann, 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*

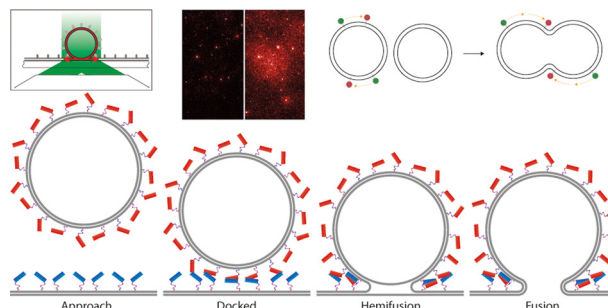


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13019

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

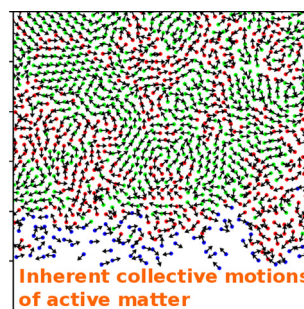
Guus van der Borg, Niek Crone, Aimee L. Boyle, Alexander Kros and Wouter H. Roos*



13027

The coherent motions of thermal active Brownian particles

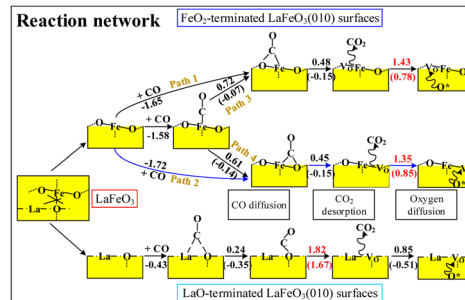
Cheng Yang, Ying Zeng, Shun Xu* and Xin Zhou*



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

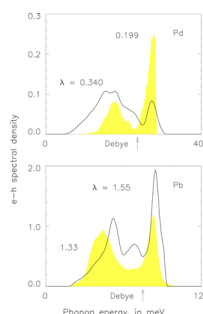
Coverage-dependent adsorption and dissociation of H₂O on Al surfaces

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



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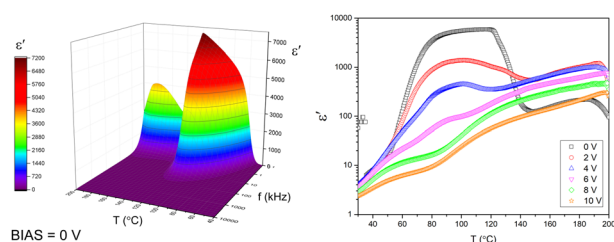
13049



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

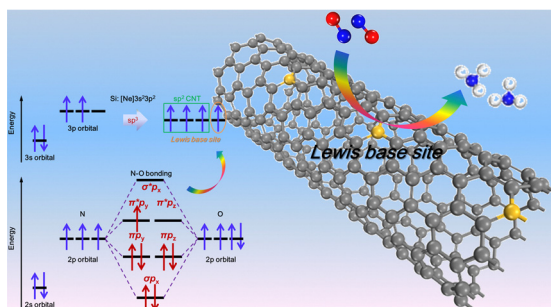
13061



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

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

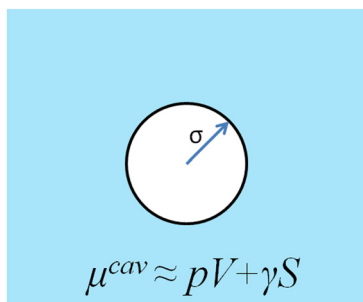
13072



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

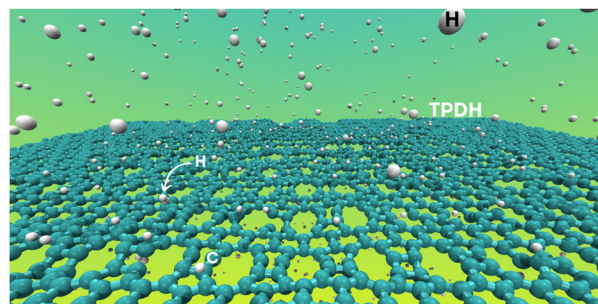


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13088

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

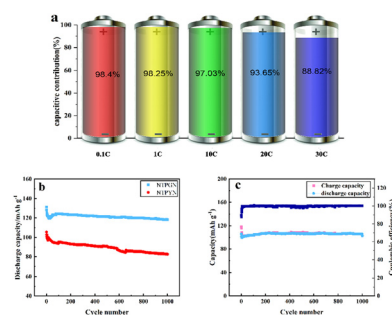
Caique C. Oliveira, Matheus Medina, Douglas S. Galvao and Pedro A. S. Autreto*



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

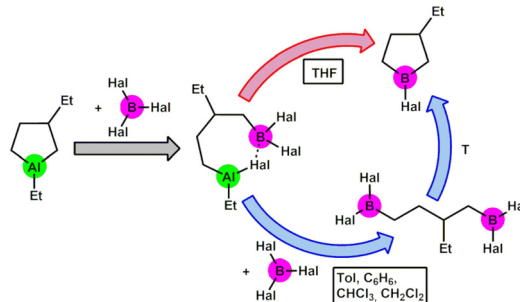
Shuang Ding, Huijin Li, Jie Yuan,* Xianli Yuan and Min Li



13104

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

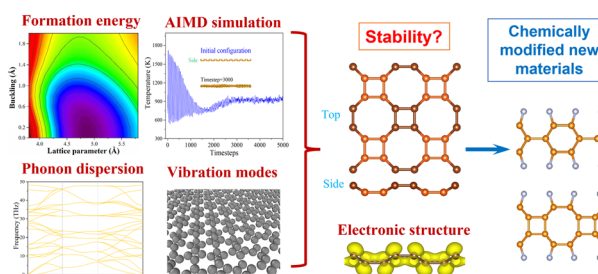
T. V. Tyumkina,* L. I. Tulyabaeva, S. M. Idrisova, D. N. Islamov, L. M. Khalilov and U. M. Dzhemilev



13116

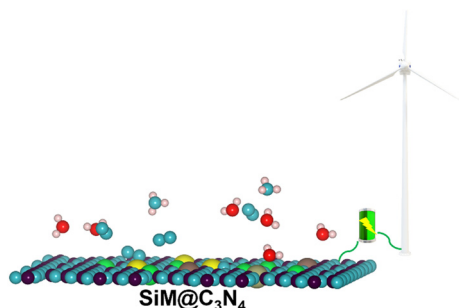
Theoretical insights into the stability of buckled tetragonal graphene and the prediction of novel carbon allotropes

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



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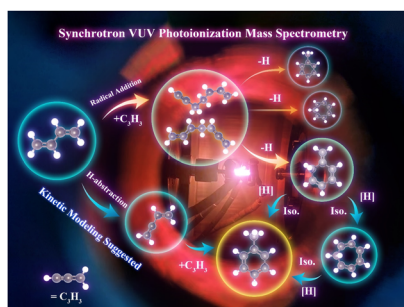
13126



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

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

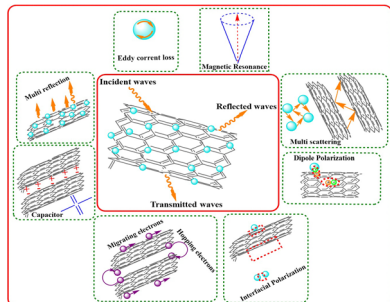
13136



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*

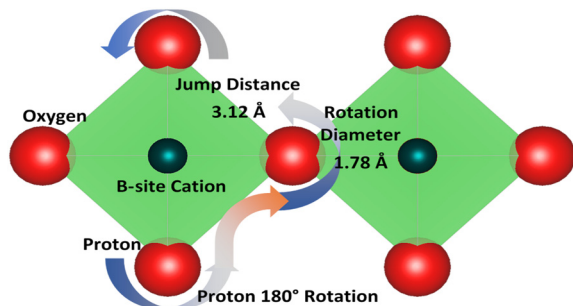
13145



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

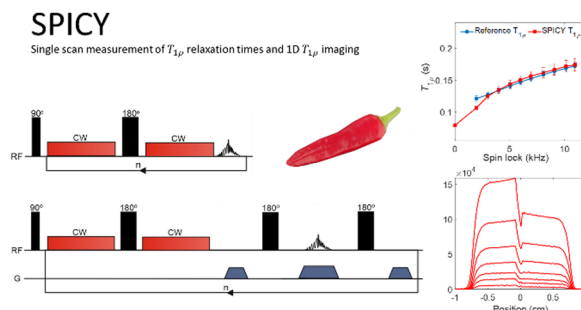


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13164

SPICY: a method for single scan rotating frame relaxometry

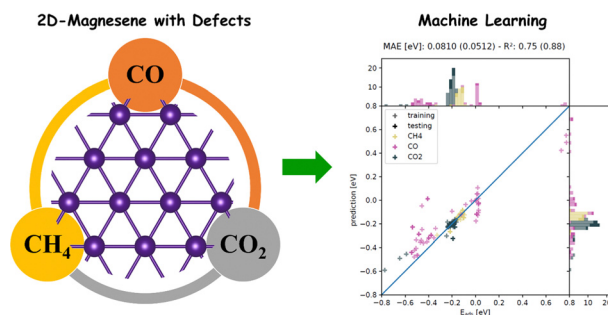
Katja Tolkkinen, Sarah E. Mailhot, Anne Selent, Otto Mankinen, Henning Henschel, Miika T. Nieminen, Matti Hanni, Anu M. Kantola, Timo Liimatainen and Ville-Veikko Telkki*



13170

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

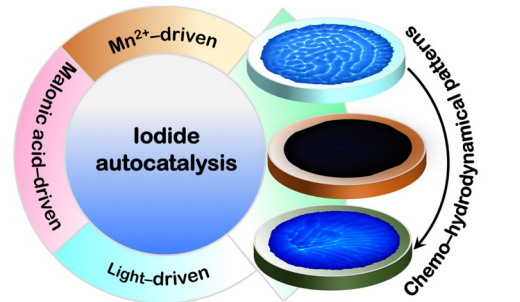
Siby Thomas,* Felix Mayr, Ajith Kulangara Madam and Alessio Gagliardi*



13183

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

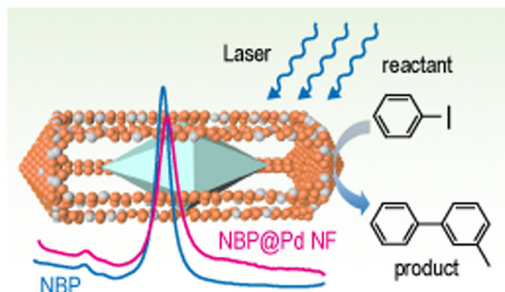
Ling Yuan,* Hongzhang Wang, Chunxiao Meng, Zhenfang Cheng, Xiaoli Lv and Qingyu Gao*



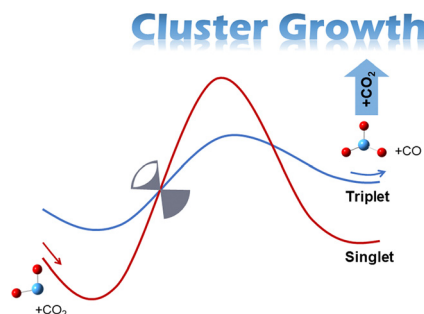
13189

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*

