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REVIEWS

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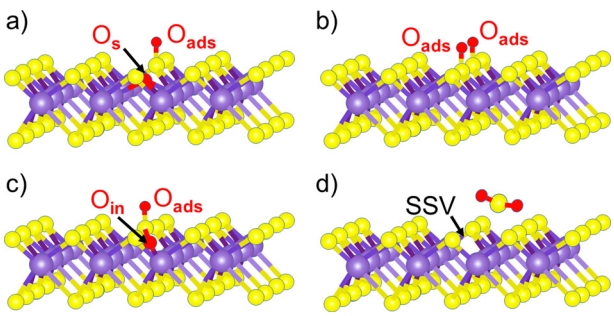
A brief review on thermally induced oxidation and oxidative etching of thin MoS_2 crystals

Robert Szoszkiewicz



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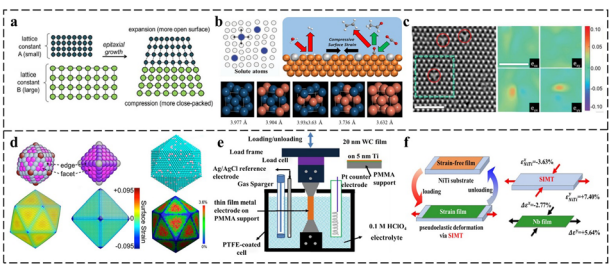
Atomic understanding of the strain-induced electrocatalysis from DFT calculation: progress and perspective

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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REVIEWS

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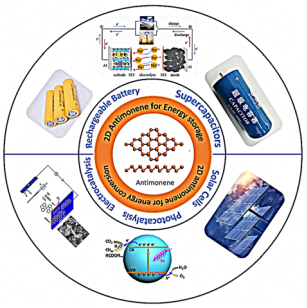
Research progress of two-dimensional antimonene in energy storage and conversion

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



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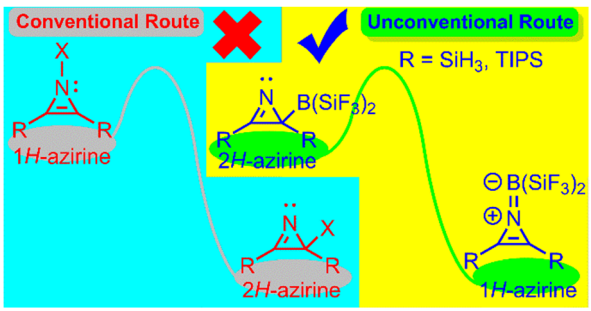
An unprecedented route to achieve persistent 1*H*-azirine

Alvi Muhammad Rouf* and Jun Zhu*



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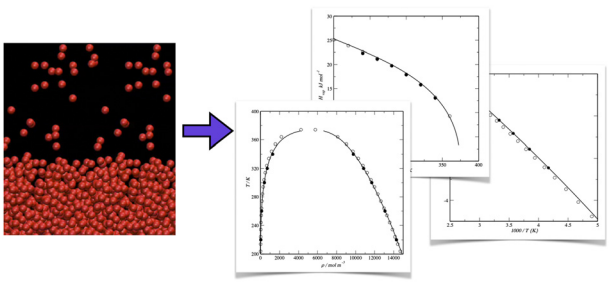
Molecular modelling of the thermophysical properties of fluids: expectations, limitations, gaps and opportunities

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



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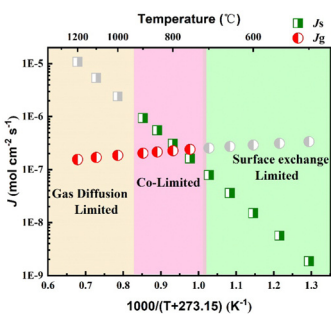
Perspective on high-temperature surface oxygen exchange in a porous mixed ionic-electronic conductor for solid oxide cells

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



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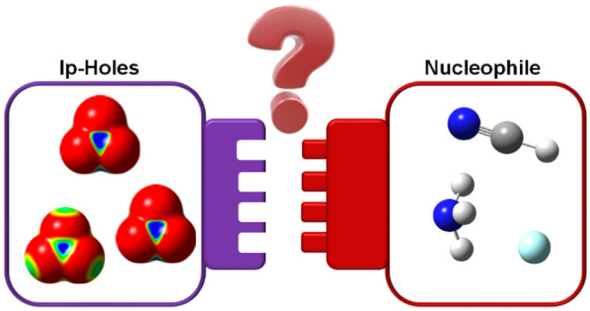

Yet another perspective on hole interactions, part II: lp-hole *vs.* lp-hole interactions

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

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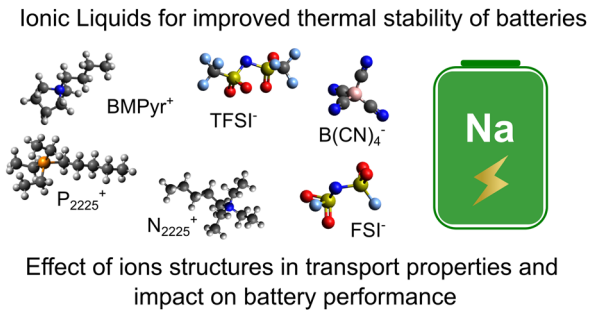

Ionic liquids as potential electrolytes for sodium-ion batteries: an overview

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

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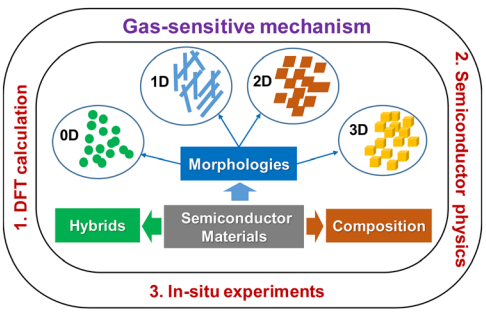

Research progress and prospects on gas-sensitive mechanisms of semiconductor sensors

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

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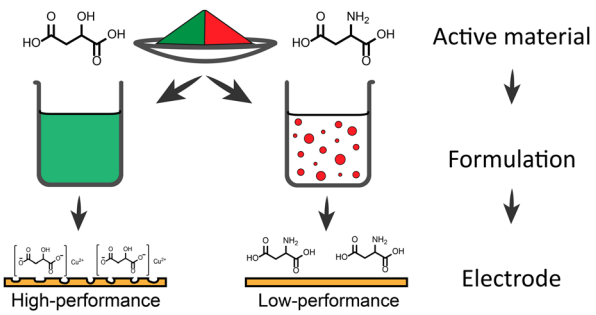

***In situ* synthesis of Cu(II) dicarboxylate metal organic frameworks (MOFs) and their application as battery materials**

Matthew Teusner, Jitendra Mata and Neeraj Sharma*

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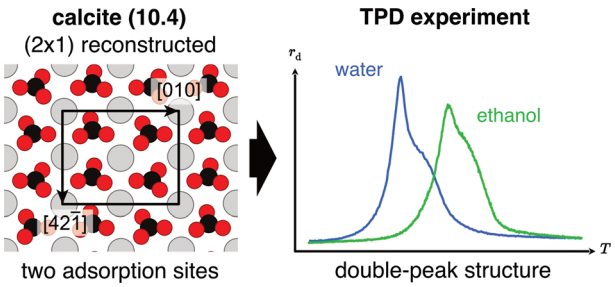

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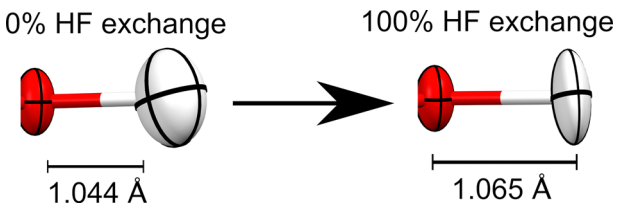
How do density functionals affect the Hirshfeld atom refinement?

Bruno Landeros-Rivera,* David Ramírez-Palma, Fernando Cortés-Guzmán, Paulina M. Dominiak and Julia Contreras-García*



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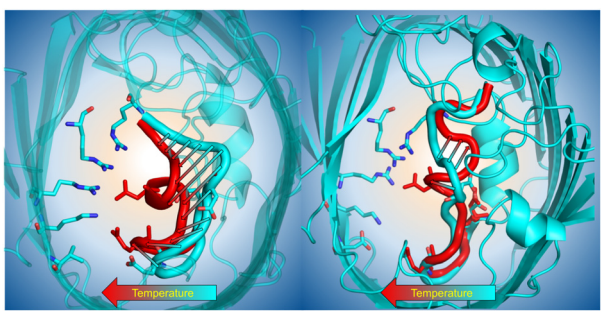
How the physical properties of bacterial porins match environmental conditions

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



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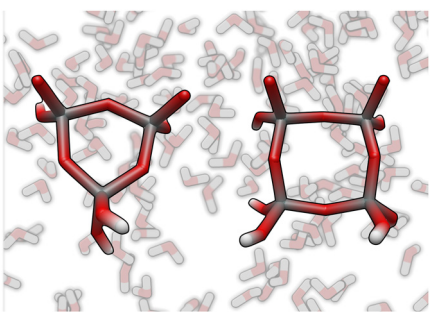
Insight into the role of excess hydroxide ions in silicate condensation reactions

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



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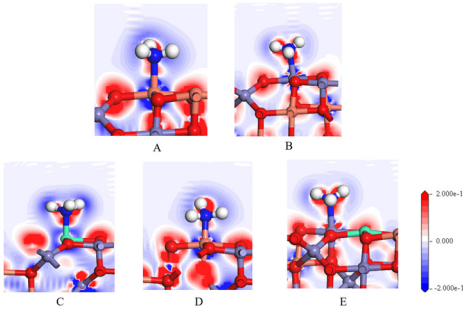

Study on the mechanism of NO_x reduction by NH_3-SCR over a $Zn_xCu_{1-x}Fe_2O_4$ catalyst

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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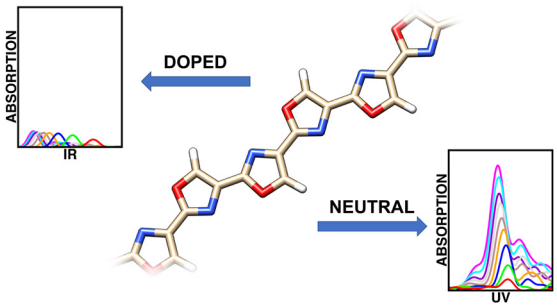

First-principles study of electronic and optical properties in 1-dimensional oligomeric derivatives of telomestatin

Joëlle Mérgola-Greef and Bruce F. Milne*

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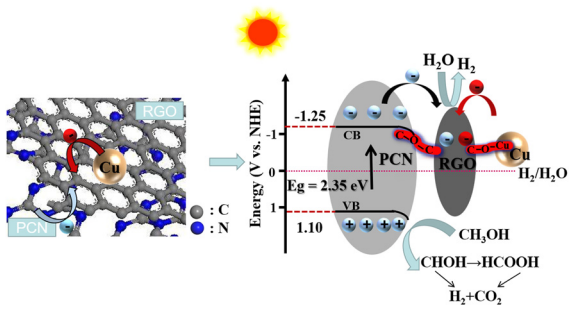

Enhanced plasmonic photocatalytic performance of C_3N_4/Cu by the introduction of a reduced graphene oxide interlayer

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

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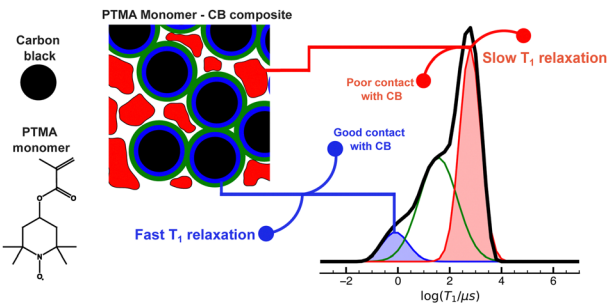

Laplace inverted pulsed EPR relaxation to study contact between active material and carbon black in Li–organic battery cathodes

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

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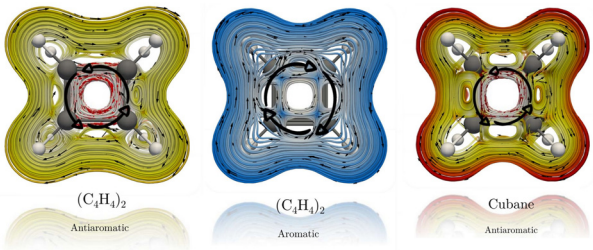
On the antiaromatic–aromatic–antiaromatic transition of the stacked cyclobutadiene dimer

Mesías Orozco-Ic* and Dage Sundholm*



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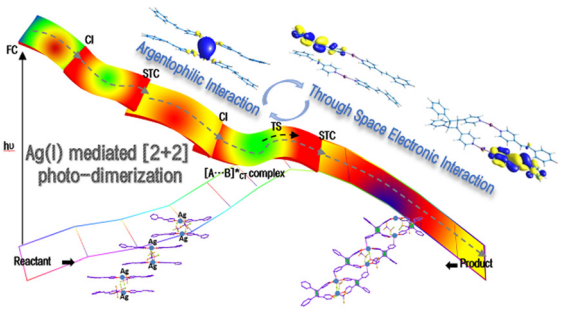
Synergetic argentophilic and through space electronic interactions in a single-crystal-to-single-crystal photocycloaddition reaction: a mechanistic study

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



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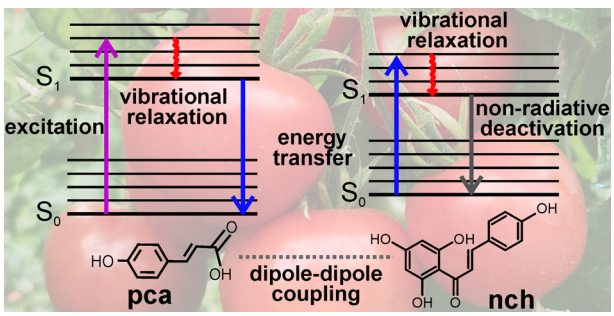
Synergic photoprotection of phenolic compounds present in tomato fruit cuticle: a spectroscopic investigation in solution

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



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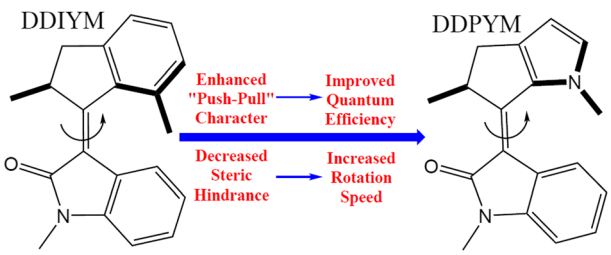
Simultaneously improving the efficiencies of photo- and thermal isomerization of an oxindole-based light-driven molecular rotary motor by a structural redesign

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



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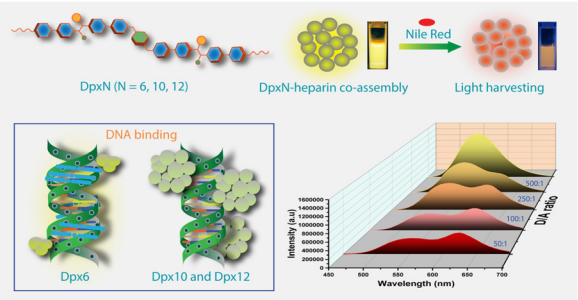

Contrasting luminescence in heparin and DNA-templated co-assemblies of dimeric cyanostilbenes: efficient energy transfer in heparin-based co-assemblies

Dhananjoy Maity, Shubhra Kanti Bhaumik and Supratim Banerjee*

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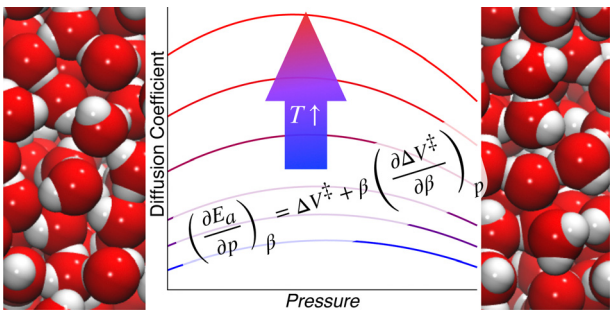

A Maxwell relation for dynamical timescales with application to the pressure and temperature dependence of water self-diffusion and shear viscosity

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

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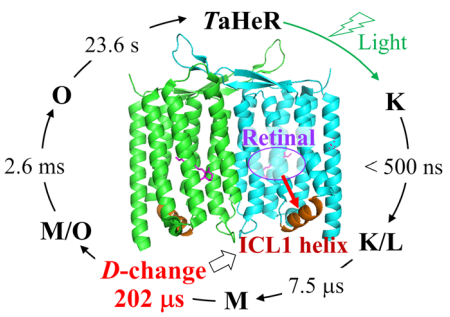
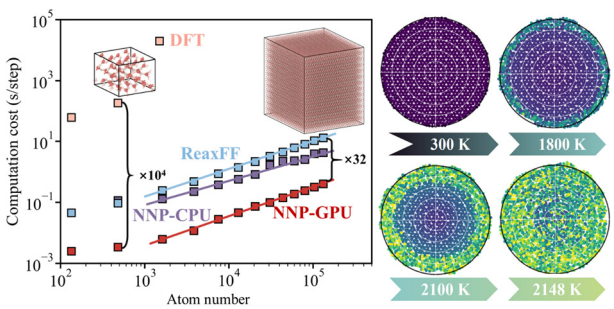


Time-resolved detection of light-induced conformational changes of heliorhodopsin

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

12841



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

Xiaoya Chang, Qingzhao Chu and Dongping Chen*

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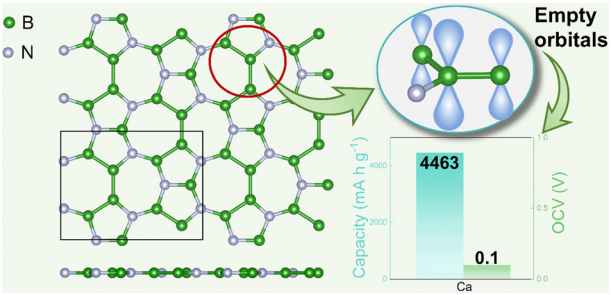
12854

B_5N_3 as a potential high-capacity electrode material for calcium ion batteries

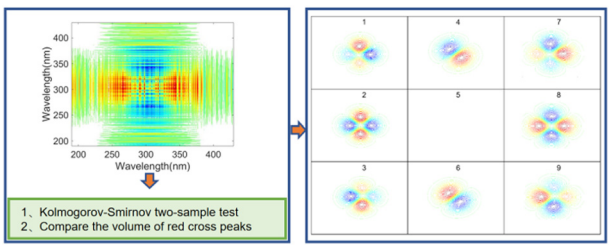
Yu Xiong, Ninggui Ma, Yuhang Wang, Tairan Wang, Shuang Luo and Jun Fan*



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

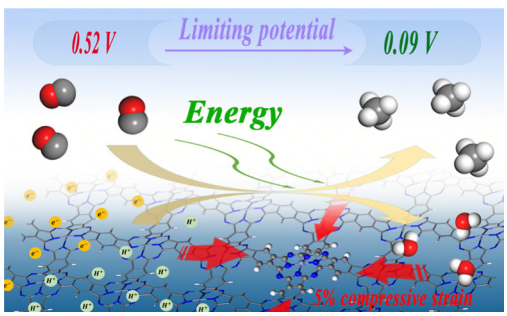
Linchen Xie, Ran Guo, Limin Yang,* Yukihiro Ozaki, Isao Noda, Yizhuang Xu* and Kun Huang*



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*



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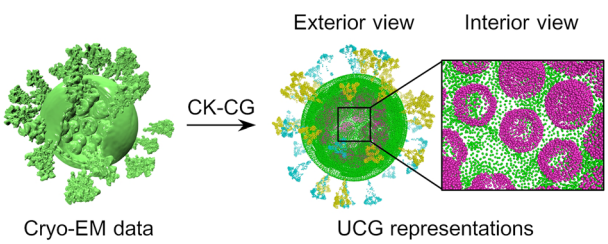
Development of multiscale ultra-coarse-grained models for the SARS-CoV-2 virion from cryo-electron microscopy data

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



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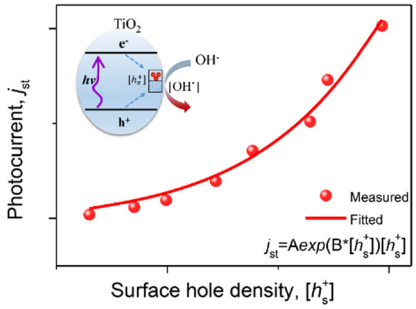
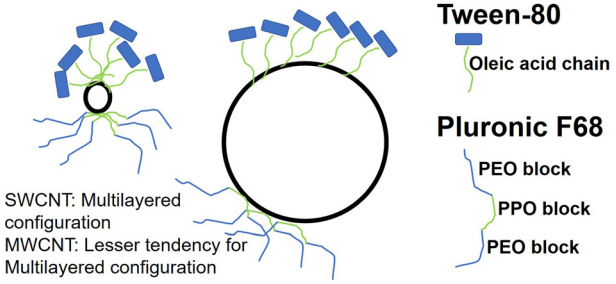
12891



Unconventional rate law of water photooxidation at TiO_2 electrodes

Shufeng Zhang,* Wenhua Leng and Kai Liu*

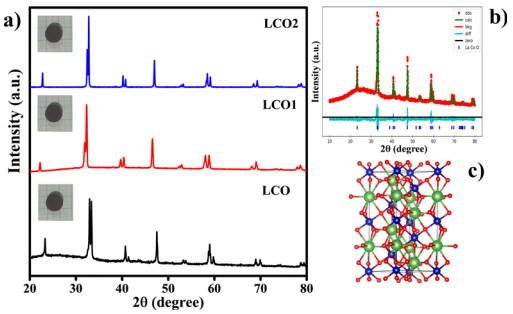
12900



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

Raman Preet Singh* and Taranpreet Kaur

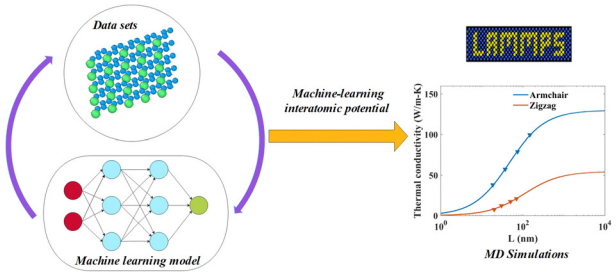
12914



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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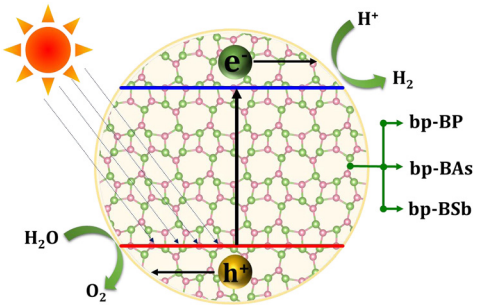
12934

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

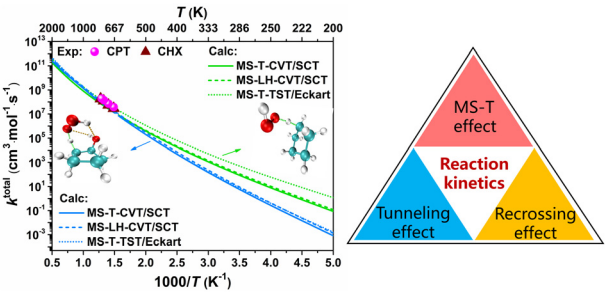
Naga Venkateswara Rao Nulakani and T. J. Dhilip Kumar*



12943

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

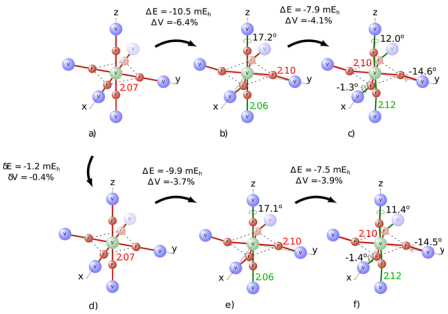
Mo Yang and Juan Wang*



12961

The role of the A monovalent cation in the AVF_3 perovskite series. A quantum mechanical investigation

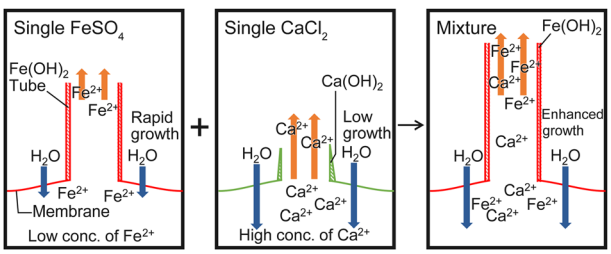
Fabien Pascale,* Neveen I. Atallah, Khaled E. El-Kelany,* Klaus Doll and Roberto Dovesi



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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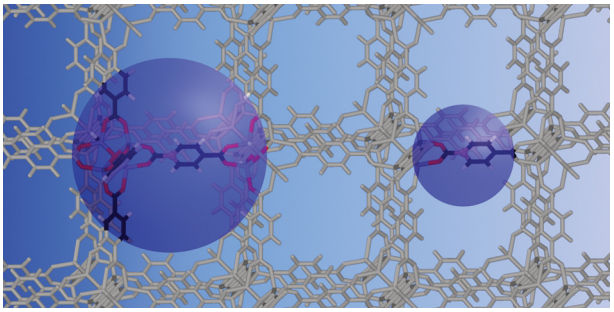
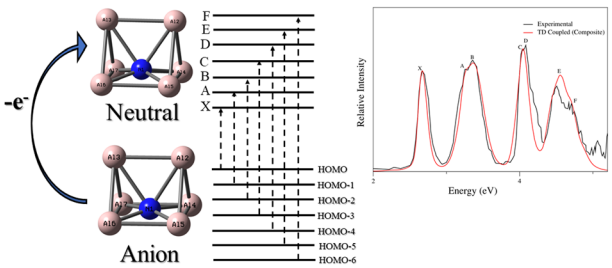
12979



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

Marius Herbold and Jörg Behler*

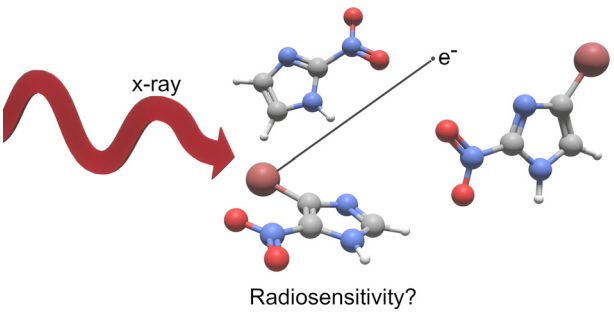
12990



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*

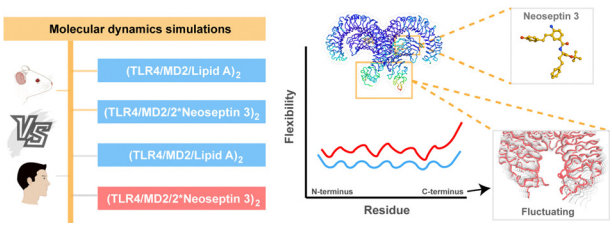
13004



Photodissociation of bromine-substituted nitroimidazole radiosensitizers

Lassi Pihlava,* Marta Berholts, Johannes Niskanen, Anton Vladyka, Kuno Kooser, Christian Stråhlman, 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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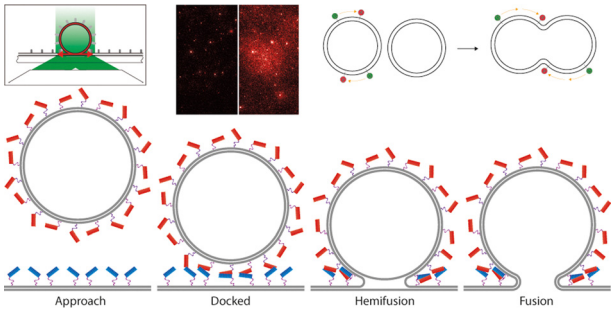
13019

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

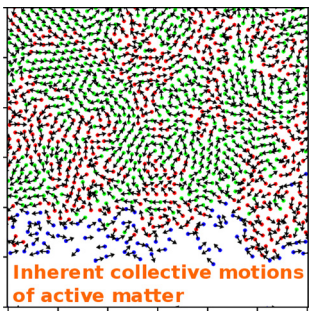
Guus van der Borg, Niek Crone, Aimee L. Boyle, Alexander Kros and Wouter H. Roos*



13027

The coherent motions of thermal active Brownian particles

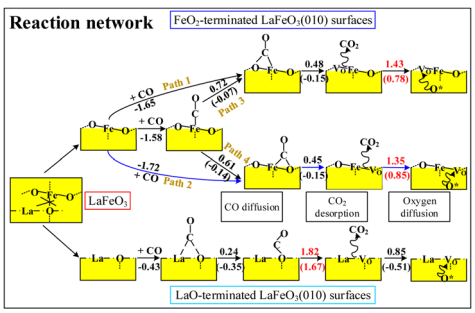
Cheng Yang, Ying Zeng, Shun Xu* and Xin Zhou*



13033

Exploration of the reaction mechanism of the $LaFeO_3$ oxygen carrier for chemical-looping steam methane reforming: a DFT study

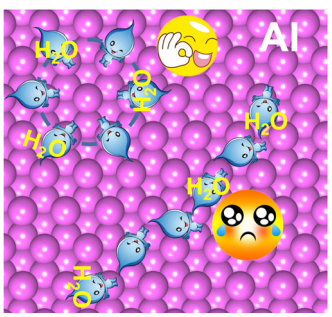
Yuchuan Feng, Xiude Hu, Xin Guo and Nana Wang*



13041

Coverage-dependent adsorption and dissociation of H_2O on Al surfaces

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



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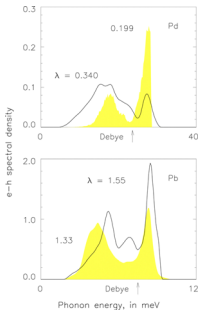
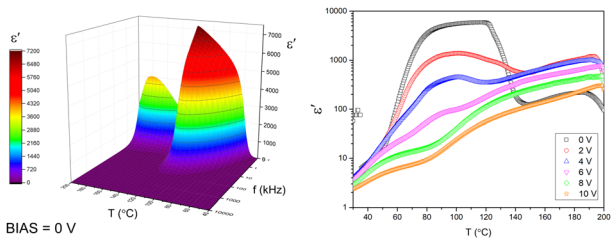


On the use of Monkhorst–Pack scheme to evaluate superconductivity and the issue of umklapp electron–phonon interactions

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

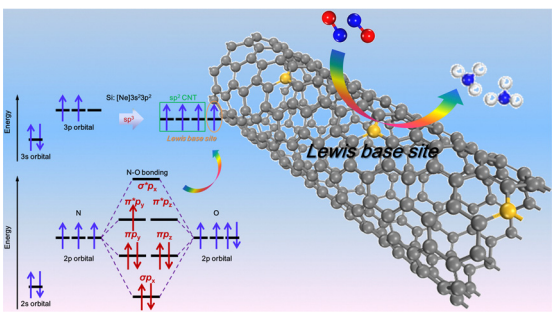
13061



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

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

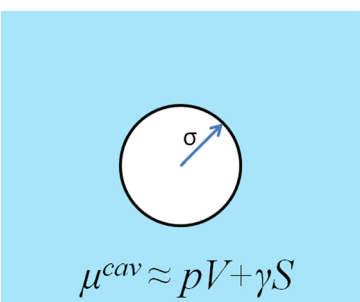
13072



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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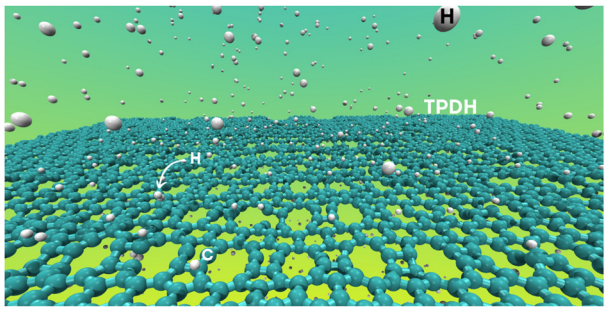
13088

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

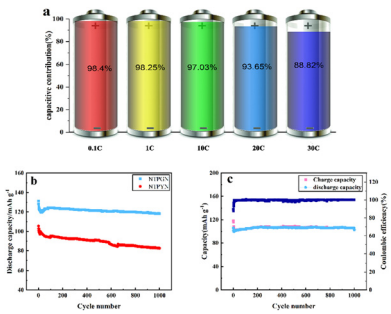
Caique C. Oliveira, Matheus Medina, Douglas S. Galvao and Pedro A. S. Autreto*



13094

N-modified carbon-coated $NaTi_2(PO_4)_3$ as an anode with high capacity and long lifetime for sodium-ion batteries

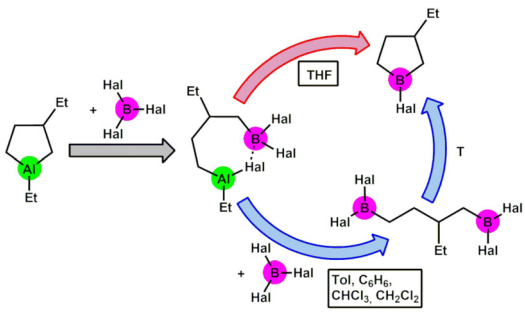
Shuang Ding, Huijin Li, Jie Yuan,* Xianli Yuan and Min Li



13104

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

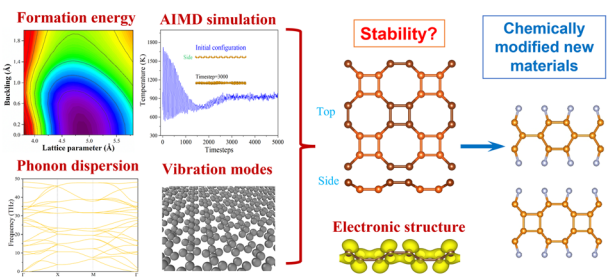
T. V. Tyumkina,* L. I. Tulyabaeva, S. M. Idrisova, D. N. Islamov, L. M. Khalilov and U. M. Dzhemilev



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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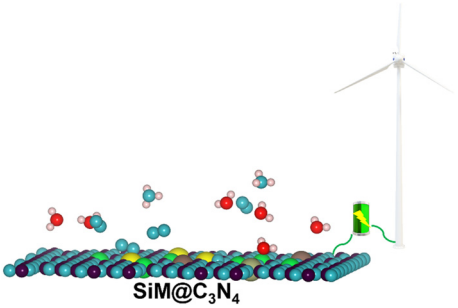
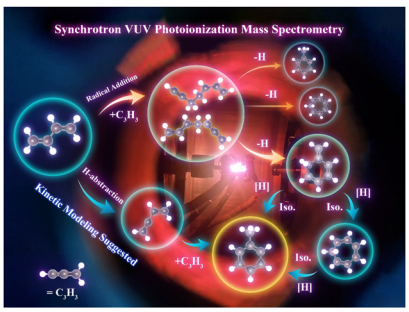


Efficient asymmetrical silicon–metal dimer electrocatalysts for the nitrogen reduction reaction

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

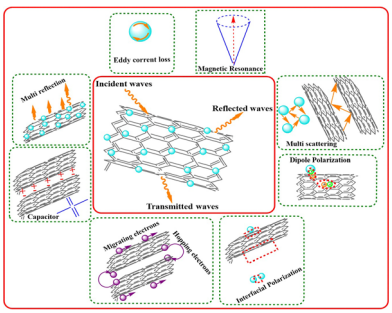
13136



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*

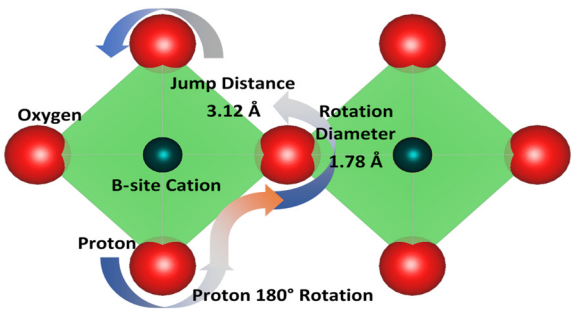
13145



Superior microwave absorption ability of $CuFe_2O_4$/MWCNT at whole Ku-band and half X-band

Mahla Tahamipoor and Hoda Hekmatara*

13155



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

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

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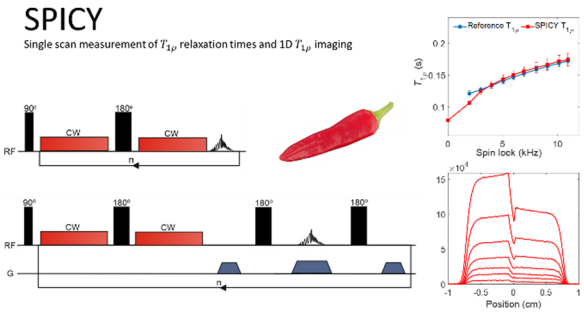
13164

SPICY: a method for single scan rotating frame relaxometry

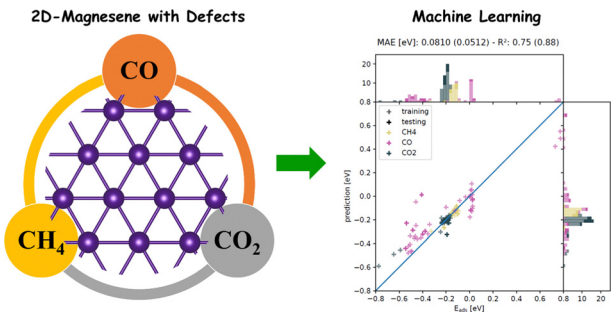
Katja Tolkkinen, Sarah E. Mailhiot, Anne Selent, Otto Mankinen, Henning Henschel, Miika T. Nieminen, Matti Hanni, Anu M. Kantola, Timo Liimatainen and Ville-Veikko Telkki*



13170

Machine learning and DFT investigation of CO, CO_2 and CH_4 adsorption on pristine and defective two-dimensional magnesene

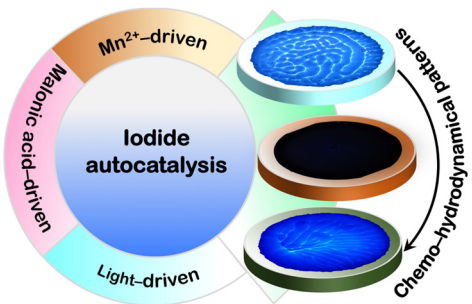
Siby Thomas,* Felix Mayr, Ajith Kulangara Madam and Alessio Gagliardi*



13183

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

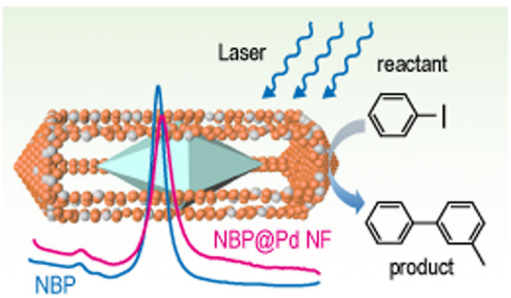
Ling Yuan,* Hongzhang Wang, Chunxiao Meng, Zhenfang Cheng, Xiaoli Lv and Qingyu Gao*



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*



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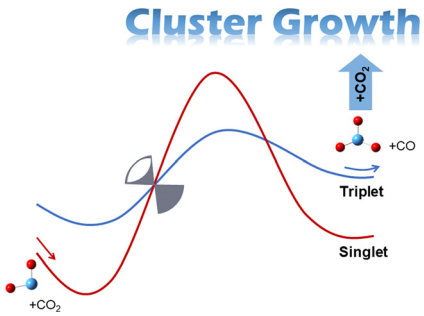

Infrared photodissociation spectroscopy of mass-selected $[TaO_3(CO_2)_n]^+$ (n = 2–5) complexes in the gas phase

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