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Cover

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Inside cover

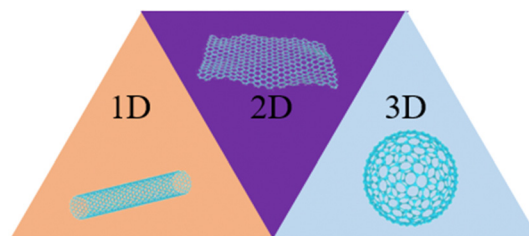
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REVIEW

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Metal–organic framework-derived metal oxides for resistive gas sensing: a review

Luyu Wang,* Jia Song and Chunyang Yu



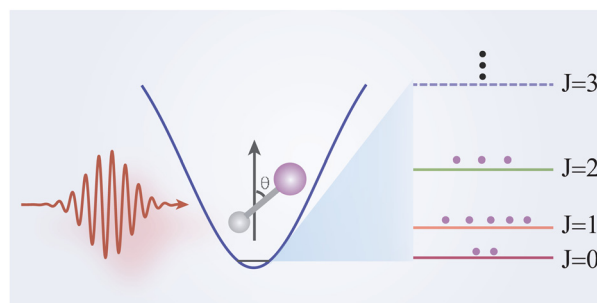
MOFs derived metal oxides for resistive gas sensing

PERSPECTIVES

32763

Quantum control of field-free molecular orientation

Qian-Qian Hong, Zhen-Zhong Lian, Chuan-Cun Shu* and Niels E. Henriksen



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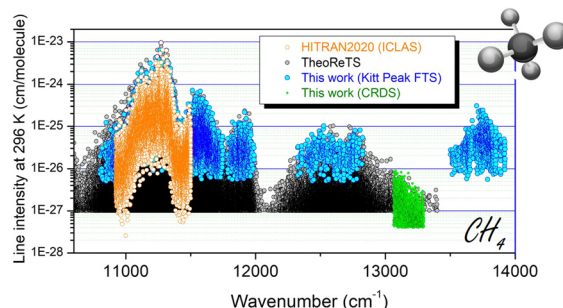


PERSPECTIVES

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The high resolution absorption spectrum of methane in the 10 800–14 000 cm⁻¹ region: literature review, new results and perspectives

A. Campargue,* E. V. Karlovets, S. S. Vasilchenko and M. Turbet

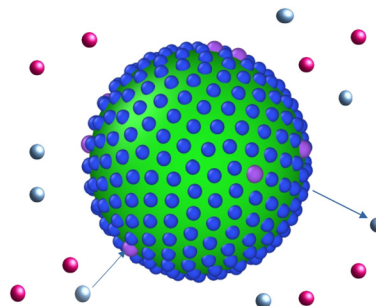


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Canonical titration simulations

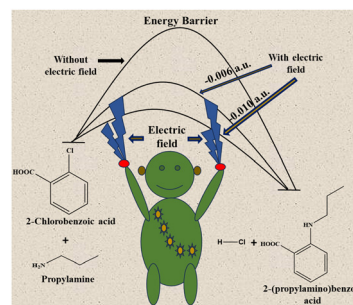
Amin Bakhshandeh and Yan Levin*



32807

External electric field, a potential catalyst for C–N cross-coupling reaction

Priyanka Yadav and Pradeep Kumar*

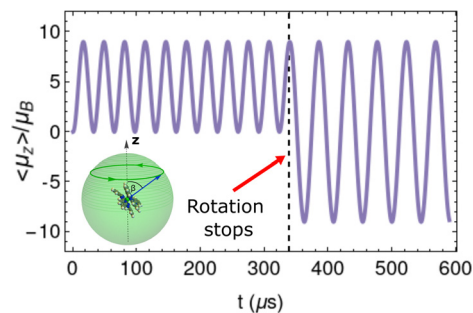


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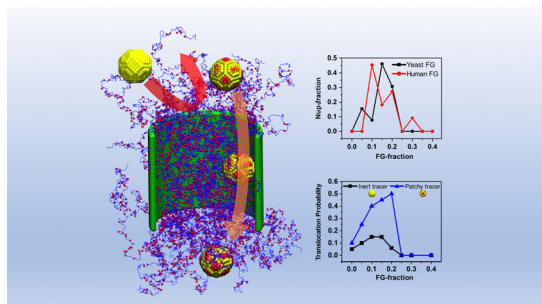
Triggering single-molecule qubit spin dynamics via non-Abelian geometric phase effects

Kieran Hymas and Alessandro Soncini*



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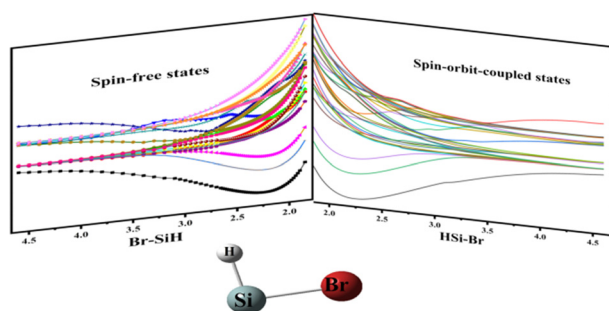
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Emergence of selectivity and specificity in a coarse-grained model of the nuclear pore complex with sequence-agnostic FG-Nups

Manoj K. Patel, Buddhapriya Chakrabarti and Ajay S. Panwar*

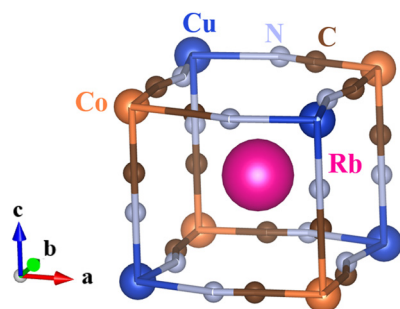
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Electronic excited states of monobromosilylene molecules including the spin-orbit-coupling

Lili Bian, Shimin Shan, Yi Lian, Lidan Xiao, Di Liu, Hang Lv,* Haifeng Xu* and Bing Yan*

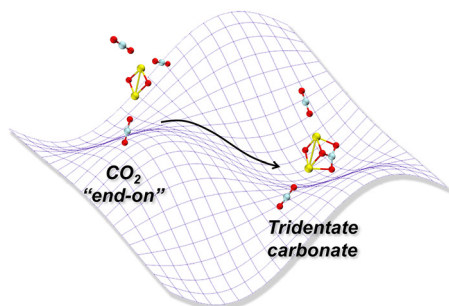
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The uniaxial zero thermal expansion and zero linear compressibility in distorted Prussian blue analogue $\text{RbCuCo}(\text{CN})_6$

Lei Wang,* Ya-Ning Sun, Xian-Deng Wei, Meng Yin, Ying Chen, Hideo Miura, Ken Suzuki and Cong Wang

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Carbon dioxide activation by discandium dioxide cations in the gas phase: a combined investigation of infrared photodissociation spectroscopy and DFT calculations

Pengcheng Liu, Jia Han, Yan Chen, Shun Lu, Quyan Su, Xiaoguo Zhou* and Weijun Zhang*

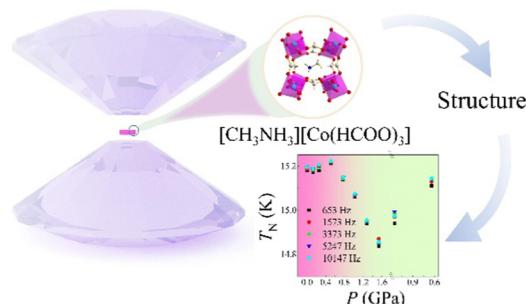


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Pressure effect on the magnetism and crystal structure of magnetoelectric metal–organic framework $[\text{CH}_3\text{NH}_3][\text{Co}(\text{HCOO})_3]$

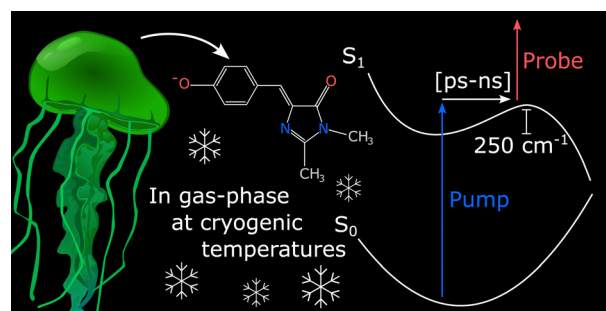
Houjian Zhou, Hao Ding, Xin Gao, Zhiwei Shen, Kun Zhai,* Bochong Wang, Congpu Mu, Fusheng Wen, Jianyong Xiang, Tianyu Xue, Yu Shu,* Lin Wang and Zhongyuan Liu*



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Excited-state dynamics and fluorescence lifetime of cryogenically cooled green fluorescent protein chromophore anions

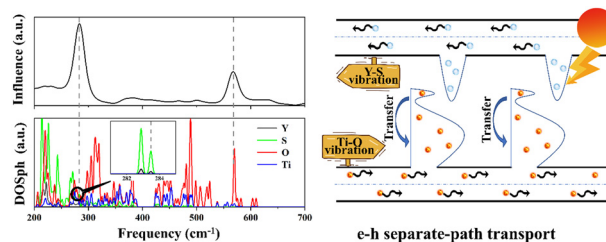
Anne P. Rasmussen, Henrik B. Pedersen and Lars H. Andersen*



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Exploration of the origin of the excellent charge-carrier dynamics in Ruddlesden–Popper oxysulfide perovskite $\text{Y}_2\text{Ti}_2\text{O}_5\text{S}_2$

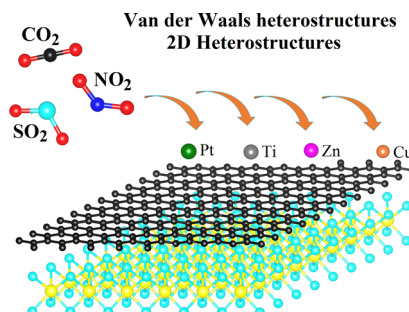
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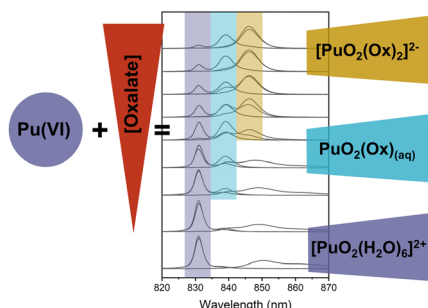
Transition metal (Ti, Cu, Zn, Pt) single-atom modified graphene/ AS_2 ($\text{A} = \text{Mo}, \text{W}$) van der Waals heterostructures for removing airborne pollutants

Erika Camarillo-Salazar, Reyes Garcia-Diaz,* Maria Teresa Romero de la Cruz, Yuliana Avila-Alvarado, H. N. Fernandez-Escamilla, Gregorio Hernández Cocoltzi and J. Guerrero-Sanchez



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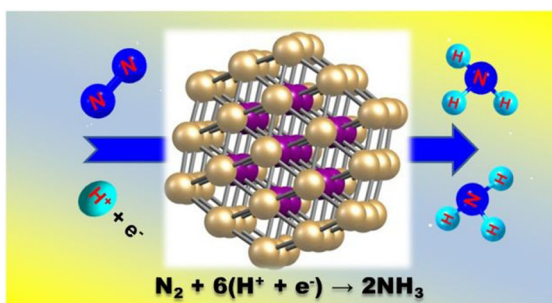
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A spectrophotometric study of the impact of pH and metal-to-ligand ratio on the speciation of the Pu(VI)-oxalate system

A. Kirstin Sockwell,* Nicole A. DiBlasi and Amy E. Hixon

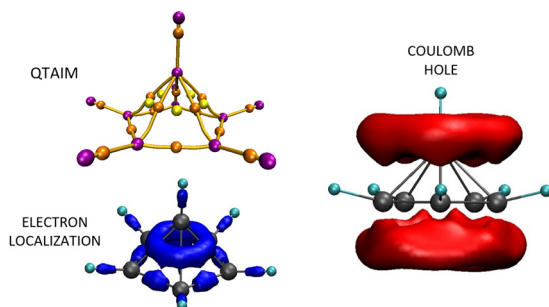
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The electrocatalytic N₂ reduction activity of core-shell iron nanoalloy catalysts: a density functional theory (DFT) study

Arunendu Das, Sandeep Das and Biswarup Pathak*

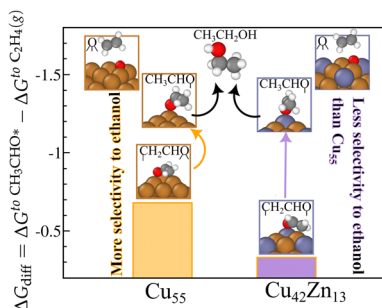
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Revisiting the bonding of the pentagonal-pyramidal C₆H₆²⁺ and C₆(CH₃)₆²⁺ dications

Luis E. Seijas,* Rafael Almeida, Luis Rincón, Cesar Zambrano, Vladimir Rodríguez, Gabriel Merino and F. Javier Torres

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Ab initio study for late steps of CO₂ and CO electroreduction: from CHCO* toward C₂ products on Cu and CuZn nanoclusters

Vivianne K. Ocampo-Restrepo, Lucas G. Verga and Juárez L. F. Da Silva*

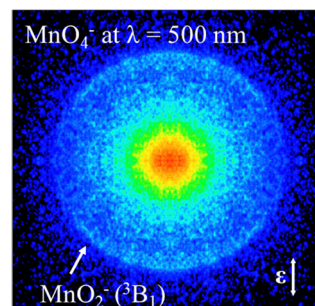


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Photodissociation of permanganate (MnO_4^-) produces the manganese dioxide anion (MnO_2^-) in an excited triplet state

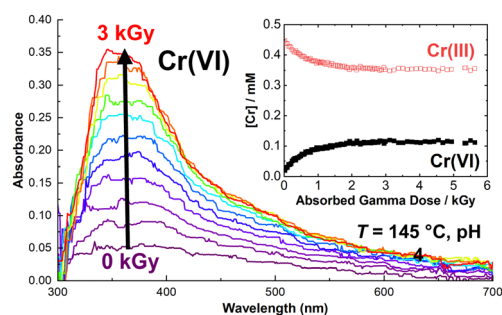
Jemma A. Gibbard,* Jonathan Reppel and Jan. R. R. Verlet



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High temperature gamma radiation-induced chromium redox chemistry *via in situ* spectroscopic measurements

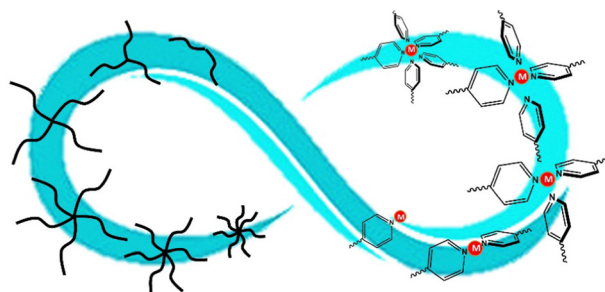
Jacy K. Conrad,* Robert V. Fox, Emma G. Danaher and Gregory P. Horne



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The network structure in transient telechelic polymer networks: extension of the Miller–Macosko model

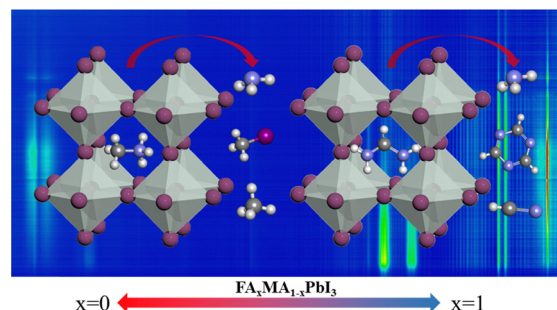
Mostafa Ahmadi,* Rosha Yazdanimoghaddam and Farhad Sharif



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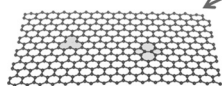
Thermal stability and decomposition kinetics of mixed-cation halide perovskites

Zicong Chen, Zhenyu Yang, Shijie Du, Dabin Lin, Fangteng Zhang, Youjun Zeng, Guanyu Liu, Zhaogang Nie* and Lin Ma*

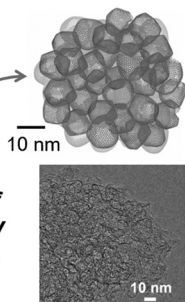


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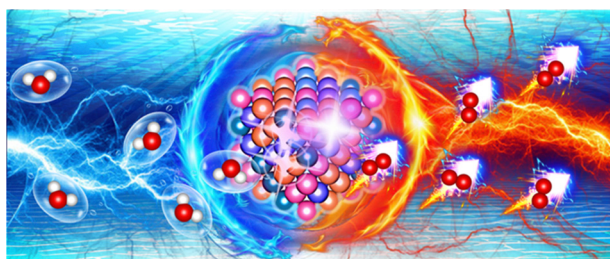
Nanoporous Graphene (NPG)

Revisited Analysis of Raman Spectroscopy coupled with XRD, TPD, nitrogen physisorption, and TEM analysis

**Surface defect healing in annealing from nanoporous carbons to nanoporous graphenes**

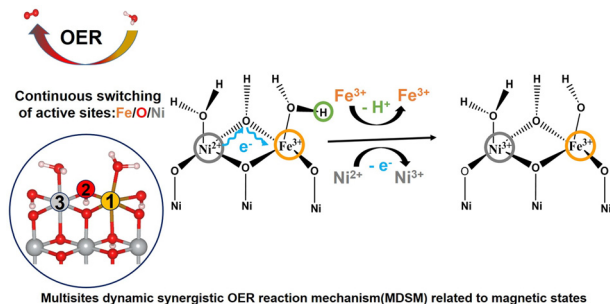
Kaoru Yamazaki,* Shunsuke Goto, Shunya Yoshino, Anna Gubarevich, Katsumi Yoshida, Hideki Kato and Masanori Yamamoto*

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**Electron-level insight into efficient synergistic oxygen evolution catalysis at multimetallic sites in PtNiFeCoCu high-entropy alloys**

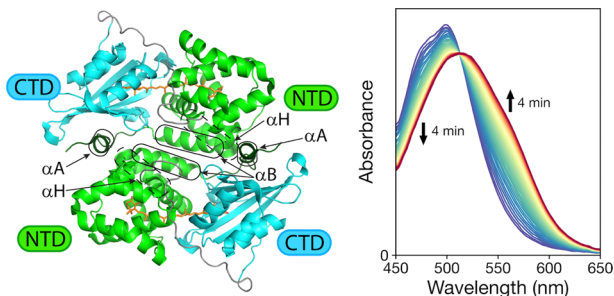
Sen Ming, Kun Meng,* Chengyi Hou, Lei Qin, Shitao Wang, Ju Rong, Xiaohua Yu and Hongying Hou*

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**A multisite dynamic synergistic oxygen evolution reaction mechanism of Fe-doped NiOOH: a first-principles study**

Hongpeng Chen, Haonan Xie, Bing Li, Jinshuo Pang, Rongrong Shi, Chen Yang, Naqin Zhao, Chunnian He, Biao Chen andENZuo Liu*

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**Photoactivation of the orange carotenoid protein requires two light-driven reactions mediated by a metastable monomeric intermediate**

Justin B. Rose, José A. Gascón, Markus Sutter, Damien I. Sheppard, Cheryl A. Kerfeld and Warren F. Beck*

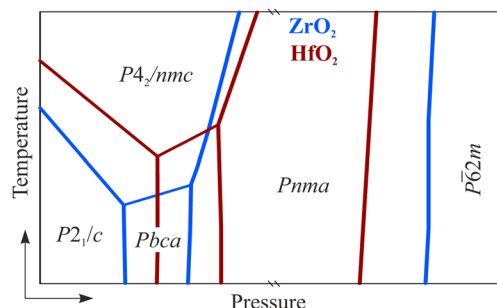


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Phase relations, thermal conductivity and elastic properties of ZrO_2 and HfO_2 polymorphs at high pressures and temperatures

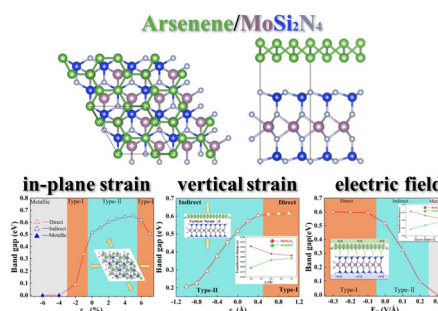
Dinara N. Sagatova,* Nursultan E. Sagatov,
Pavel N. Gavryushkin and Sergey F. Solodovnikov



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Modulating the electronic properties and band alignments of the arsenene/ MoSi_2N_4 van der Waals heterostructure via applying strain and electric field

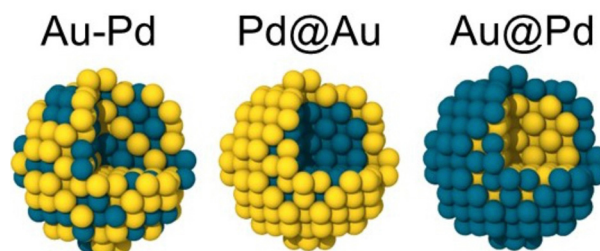
Jun Zhao,* Yunxi Qi, Can Yao and Hui Zeng*



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Tuning the surface properties of AuPd nanoparticles for adsorption of O and CO

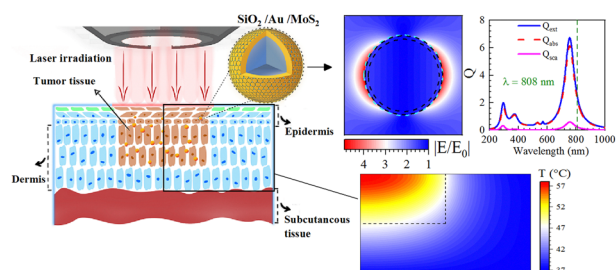
Ilya V. Chepkasov,* Ivan S. Zamulin, Viktor S. Baidyshev
and Alexander G. Kvashnin



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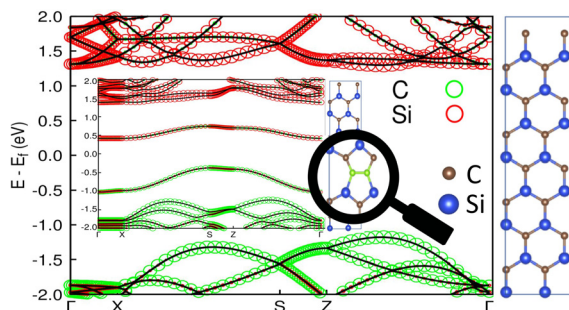
Transition metal dichalcogenide coated gold nanoshells for highly effective photothermal therapy

Saeed Bagheri, Mohsen Farokhnezhad* and
Mahdi Esmaeilzadeh*



RESEARCH PAPERS

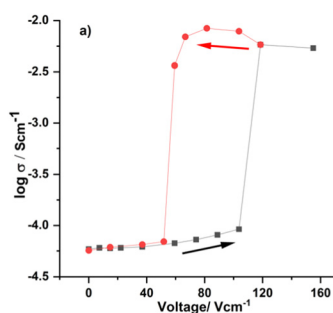
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Topological line defects in hexagonal SiC monolayer

Wallace P. Morais, Guilherme J. Inacio, Rodrigo G. Amorim, Wendel S. Paz,*
Fernando N. N. Pansini* and Fábio A. L. de Souza*

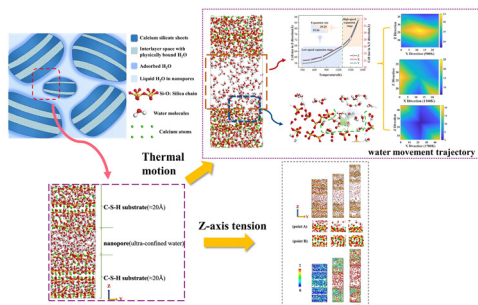
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Metal-insulator transition and resistive switching in Y-doped CeO₂ ceramics

Fawaz Almutairi, Meshari Alotaibi and Anthony R. West

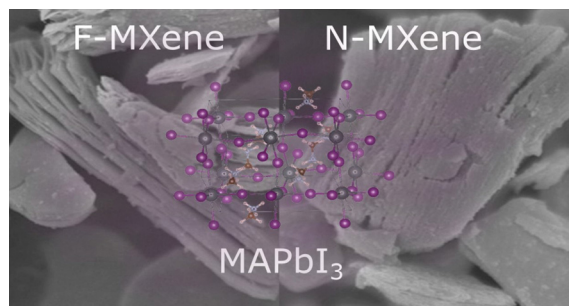
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Degradation of thermal stability and micromechanical properties of the C–S–H phase induced by ultra-confined water at elevated temperatures

Dongbo Li,* Jing Zhu, Qinlong Liu, Qinde Qi and Zhentao Bai

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Interfacial interactions of doped-Ti₃C₂ MXene/MAPbI₃ heterostructures: surfaces and the theoretical approach

Muhammad Abiyyu Kenichi Purbayanto, Arramel,*
See Wee Koh, Francesco Maddalena, Dorota Moszczyńska,
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Hong Li, Muhammad Danang Birowosuto* and
Agnieszka Maria Jastrzębska*

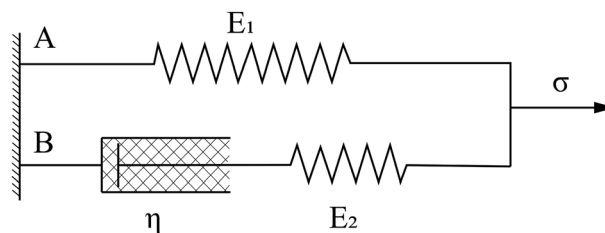


RESEARCH PAPERS

33094

A performance degradation model of nitrile butadiene rubber (NBR) O-rings for hydrogen permeation effects under high-pressure

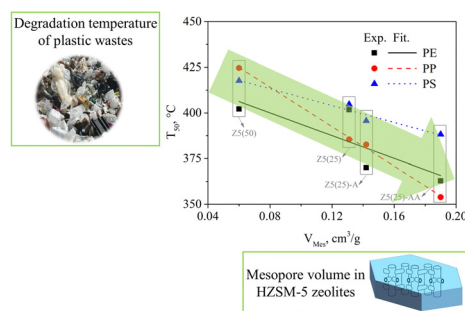
Di Wu, Yantang Li, Yang Hua, Jingxiang Xu, Xiaolu Zhang and Yang Miao*



33104

Fabrication of mesopore-rich HZSM-5 to boost the degradation of plastic wastes

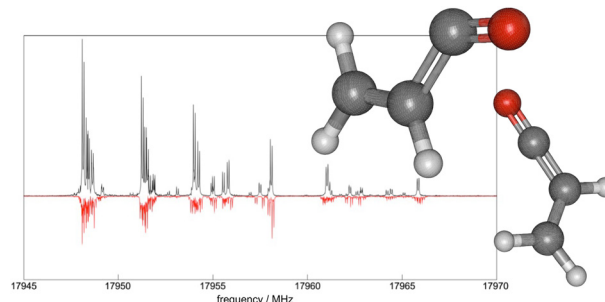
Chenggong Song, Xu Hou,* Hao Zhou, Huimin Qiao, Li Yin, Jing Huang, Enxian Yuan* and Tingting Cui*



33112

Fourier-transform microwave spectroscopy of the *s-trans*-3-propenalyl ($\text{CH}_2\text{CH}\dot{\text{C}}\text{O}$) and 3-propenolyl ($\dot{\text{C}}\text{H}_2\text{CHCO}$) radicals

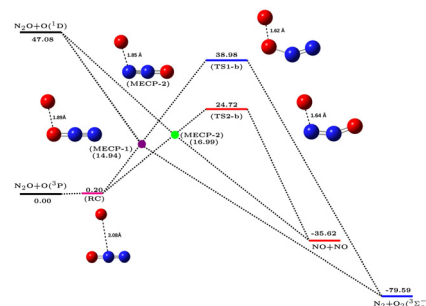
Yi-Ting Liu, Ching-Hua Chang, Masakazu Nakajima and Yasuki Endo*



33119

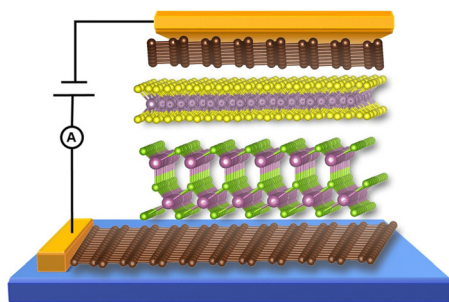
Mechanistic insight into the $\text{N}_2\text{O} + \text{O}(^1\text{D}, ^3\text{P})$ reaction: role of post-CCSD(T) corrections and non-adiabatic effects

Vishva Jeet Anand and Pradeep Kumar*



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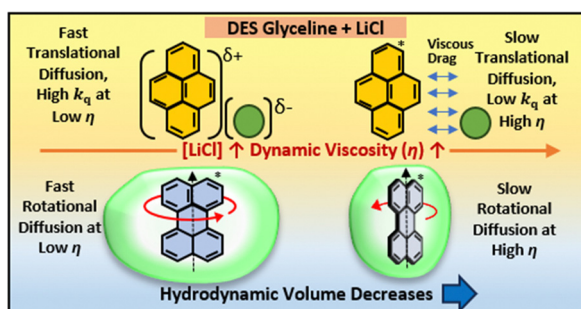
33130



The tunneling electroresistance effect in a van der Waals ferroelectric tunnel junction based on a graphene/ In_2Se_3 / MoS_2 /graphene heterostructure

Yu-Zhu Liu, Jian-Qing Dai,* Jin Yuan and Miao-Wei Zhao

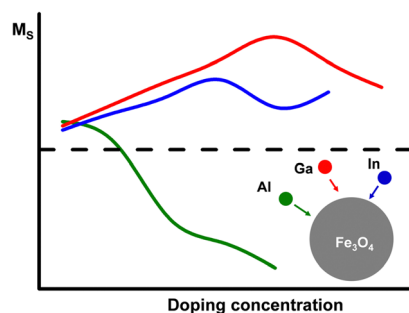
33141



Correlation of solute diffusion with dynamic viscosity in lithium salt-added (choline chloride + glycerol) deep eutectic solvents

Manish Kumar and Siddharth Pandey*

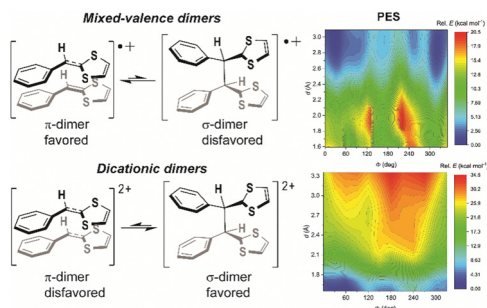
33152



Regulation of saturation magnetization of magnetite by doping with group III elements

Yanying Ren, Yanying Li, Nan Xu, Kun Guo, Zhaohui Xu, Xin Chen,* Hongsheng Liu* and Jufeng Gao

33159



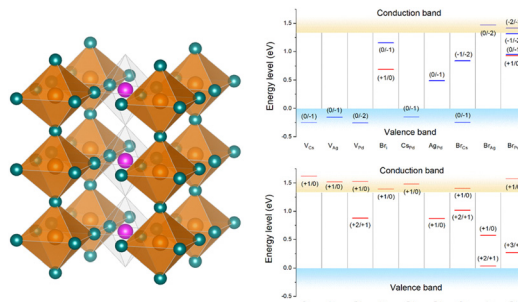
DFT investigations of phenyldithiafulvene dimers at different oxidation states

Liam H. Britt, Ramin Eradeh, Chris Leung and Yuming Zhao*



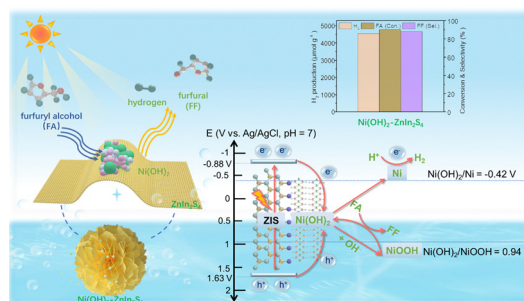
Wenjun Chu, Xinbo Ma and Zhenyu Li*

Wenjun Chu, Xinbo Ma and Zhenyu Li*



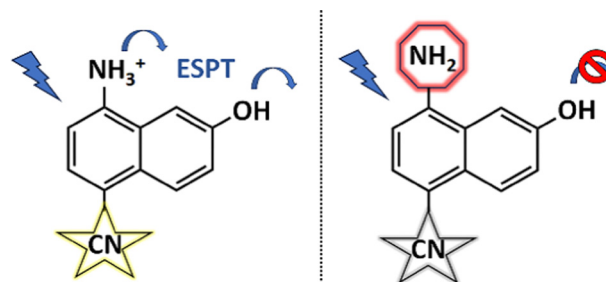
Wanqiong Kang, Fen Guo, Lei Mao, Yi Liu,* Chuang Han
and Lan Yuan*

Wanqiong Kang, Fen Guo, Lei Mao, Yi Liu,* Chuang Han
and Lan Yuan*



Jialin Xie, Rachel E. Nealon, Zelia T. Egan and
Kana Takematsu*

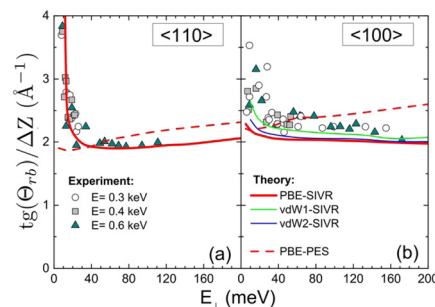
Jialin Xie, Rachel E. Nealon, Zelia T. Egan and
Kana Takematsu*



33193

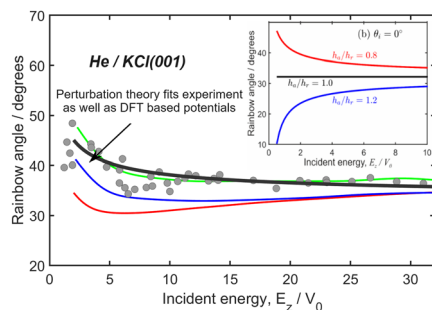
Gisela Anahí Bocan,* Hanadi Breiss, Samir Szilasi,
Anouchah Momeni, Elena Magdalena Staicu Casagrande,
Esteban Alejandro Sánchez, María Silvia Gravielle* and
Hocine Khemliche

Gisela Anahí Bocan,* Hanadi Breiss, Samir Szilasi,
Anouchah Momeni, Elena Magdalena Staicu Casagrande,
Esteban Alejandro Sánchez, María Silvia Gravielle* and
Hocine Khemliche



COMMENTS

33198



Reply to the 'Comment on "Perturbation theory of scattering for grazing-incidence fast-atom diffraction"' by G. A. Bocan, H. Breiss, S. Szilasi, A. Momeni, E. M. S. Casagrande, E. A. Sánchez, M. S. Gravielle and H. Khemliche, *Phys. Chem. Chem. Phys.*, 2023, 25, DOI: 10.1039/D3CP02486E

W. Allison,* S. Miret-Artés and E. Pollak

