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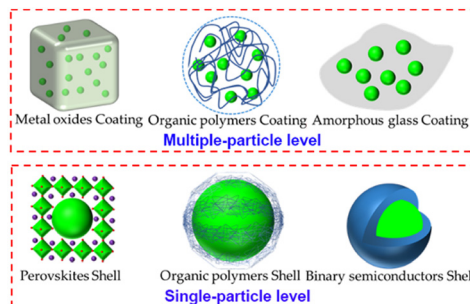
See Ying Ruan *et al.*,
pp. 17798–17807.
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Phys.*, 2023, 25, 17798.

REVIEWS

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Recent advances in encapsulation of highly stable perovskite nanocrystals and their potential applications in optoelectronic devices

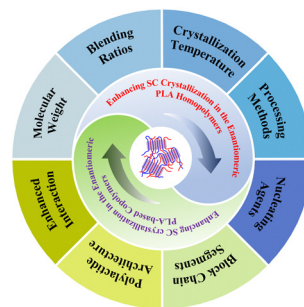
Zhengwei Cao, Feng Zhang,* Jiaqi Liu, Cuihe Fan, Yukun Wu and Yuying Hao*



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Recent advances in enhancing stereocomplexation between poly(lactide) enantiomeric chains

Mingwei Guo,* Weixin Wu, Wenjing Wu, Ruizhe Wang, Liming Huang and Qinwei Gao*



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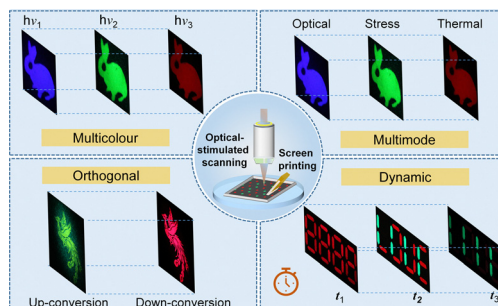


PERSPECTIVES

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Recent advances in the anti-counterfeiting applications of long persistent phosphors

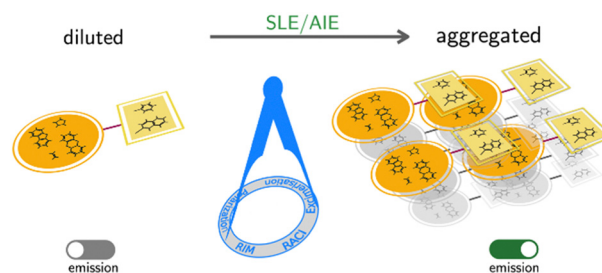
Qingqing Kuang, Xiaochun Hou, Chengxue Du, Xiaojun Wang* and Dangli Gao*



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Organic compounds for solid state luminescence enhancement/aggregation induced emission: a theoretical perspective

Michele Turelli,* Ilaria Ciofini,* Qinfan Wang, Alistar Ottochian, Frédéric Labat and Carlo Adamo*

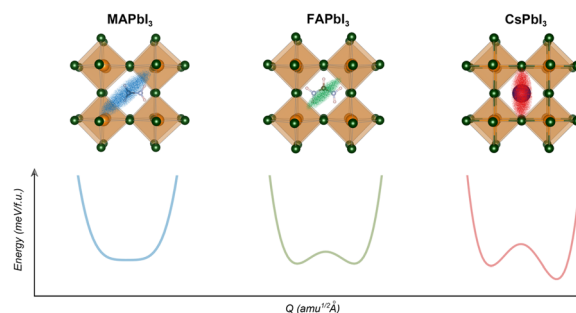


COMMUNICATIONS

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Crystal-liquid duality enhanced dynamical stability of hybrid perovskites

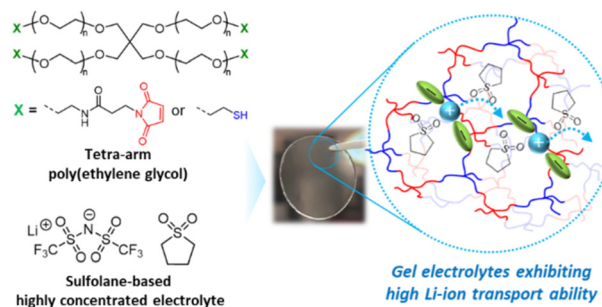
Xuan-Yan Chen, Bai-Qing Zhao, Zheng Liu, Su-Huai Wei* and Xie Zhang*



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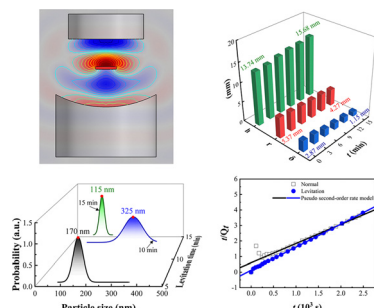
Tetra-arm poly(ethylene glycol) gels with highly concentrated sulfolane-based electrolytes exhibiting high Li-ion transference numbers

Natsumi Tasaki, Yosuke Ugata, Kei Hashimoto, Hisashi Kokubo, Kazuhide Ueno, Masayoshi Watanabe and Kaoru Dokko*



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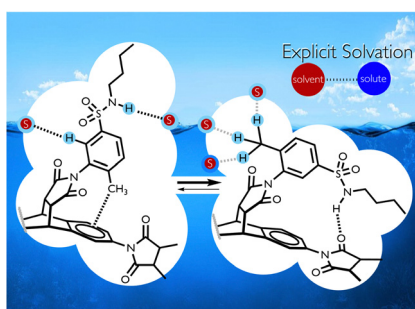
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Evaporation kinetics during containerless chemical synthesis of ZIF-8 in levitated droplets

Yuhang Zheng, Qiang Zhuang, Ying Ruan* and Bingbo Wei

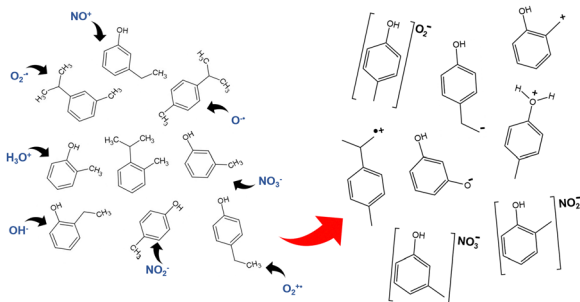
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Rationalizing hydrogen bond solvation with Kamlet-Taft LSER and molecular torsion balances

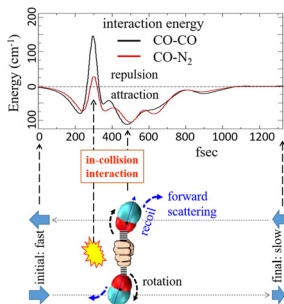
Bright U. Emenike,* Arzu Sevimler, Amiel Farshadmand and Armando J. Roman

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A SIFT-MS study of positive and negative ion chemistry of the *ortho*-, *meta*- and *para*-isomers of cymene, cresol, and ethylphenol

Stefan J Swift,* Nikola Sixtová, Maroua Omezzine Gnioua and Patrik Španěl

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Imaging rotational energy transfer: comparative stereodynamics in CO + N₂ and CO + CO inelastic scattering

Zhong-Fa Sun,* Roy J. A. Scheidsbach, Marc C. van Hemert, Ad van der Avoird, Arthur G. Suits and David H. Parker*

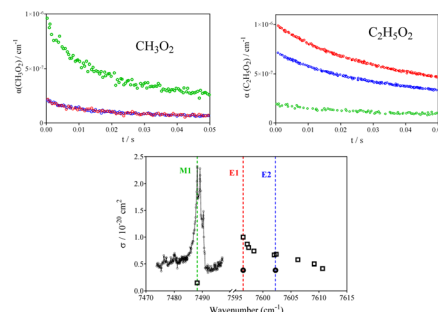


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Rate constant and branching ratio of the reaction of ethyl peroxy radicals with methyl peroxy radicals

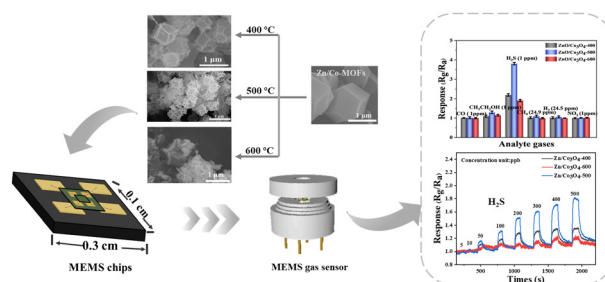
Cuihong Zhang, Chuanliang Li, Weijun Zhang, Xiaofeng Tang, Laure Pillier, Coralie Schoemaecker and Christa Fittschen*



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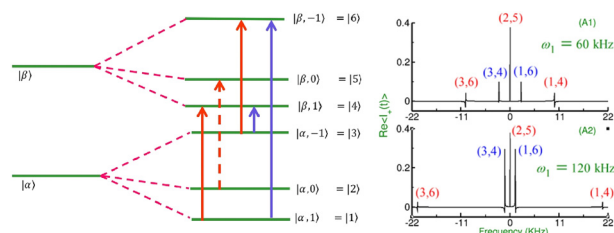
Preparation of MOF-derived ZnO/Co₃O₄ nanocages and their sensing performance toward H₂S

Han Liu, Jiawei Kong, Zhe Dong, Yongmei Zhao, Baoli An, Junping Dong, Jiaqiang Xu* and Xiaohong Wang*



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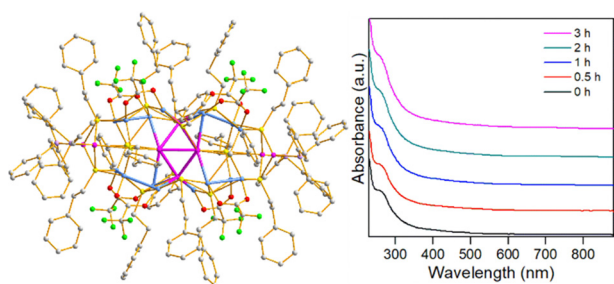
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Quantifying quadrupole effects in the NMR spectra of spin-1/2 nuclei in rotating solids

Nisha Bamola, Mohit Bansal and Ramesh Ramachandran*

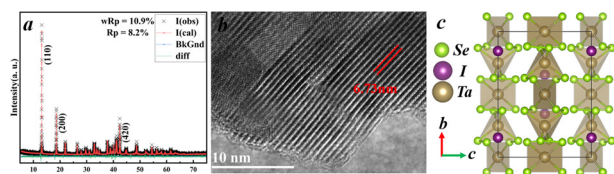
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Ag₁₀Cu₁₆ nanoclusters with triple-ligand protection: total structure and electronic structure analysis

Xueli Sun, Simin Li, Guolong Tian, Yanli Gao, Jianyu Wei* and Hui Shen*

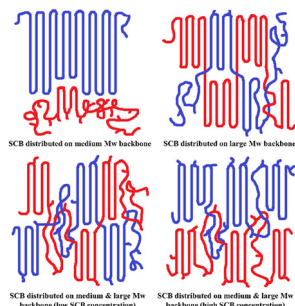
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Significantly anisotropic Raman response of the (110) surface in quasi-one-dimensional system (TaSe₄)₂ by polarized Raman spectroscopy

Xiao Gao, Pin Song, Zhongti Sun, Xuechao Li, Chuanqiang Wu and Haiping Chen*

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Unraveling the influential mechanism of short-chain branching on the crystallization of trimodal polyethylene by molecular dynamics simulation

Min Cai, Xuelian He,* Zhen Liu and Boping Liu*

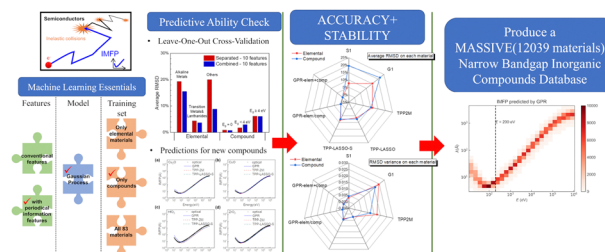


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Establishment and validation of an electron inelastic mean free path database for narrow bandgap inorganic compounds with a machine learning approach

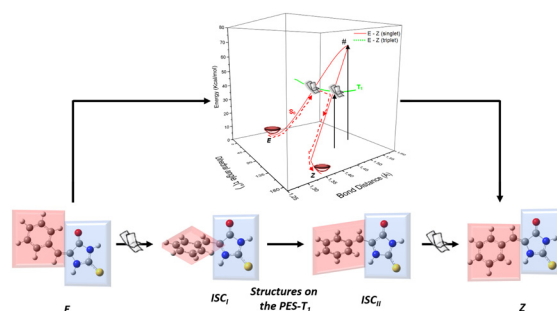
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Hideki Yoshikawa, Shigeo Tanuma, Yang Sun and
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GFP-related chromophores: photoisomerization, thermal reversion, and DNA labelling

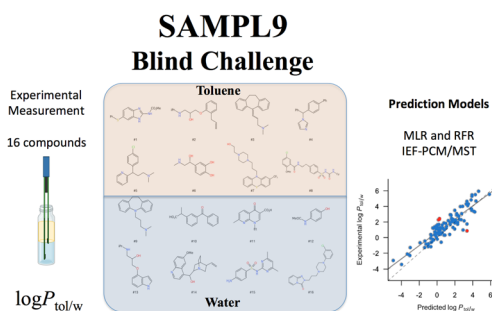
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Noelia M. Ceballos, E. Nahir Ruiz Pereyra, Lucia Lanfri,
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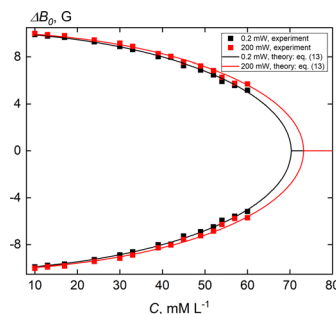
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Carles Curutchet, Laia Bisbal, Rebeca Ruiz, Clara Ràfols*
and F. Javier Luque*



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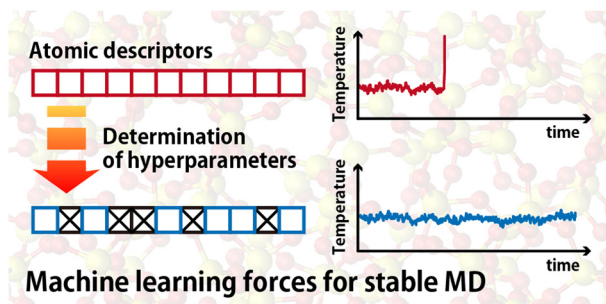
Experimental confirmation of the formation of a spin polariton in dilute solutions of paramagnetic particles

K. M. Salikhov, M. M. Bakirov, R. B. Zaripov and
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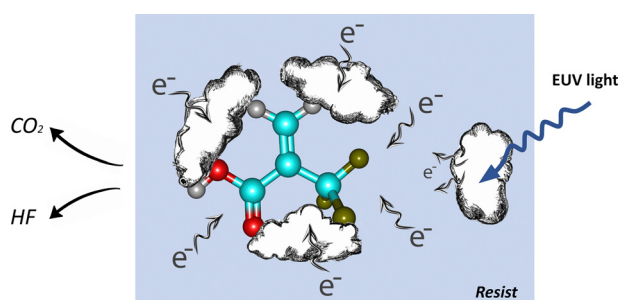
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Determination of hyper-parameters in the atomic descriptors for efficient and robust molecular dynamics simulations with machine learning forces

Jianbo Lin,* Ryo Tamura,* Yasunori Futamura, Tetsuya Sakurai and Tsuyoshi Miyazaki*

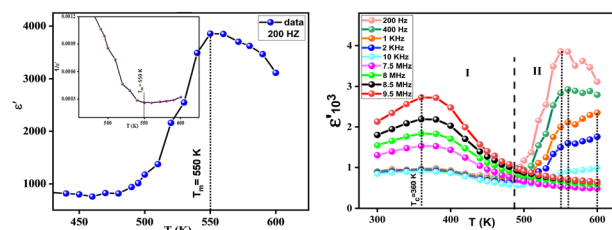
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Low-energy electron interaction with 2-(trifluoromethyl)acrylic acid, a potential component for EUVL resist material

Reza Tafrishi, Daniela Torres-Diaz, Lionel Amiaud, Anne Lafosse and Oddur Ingólfsson*

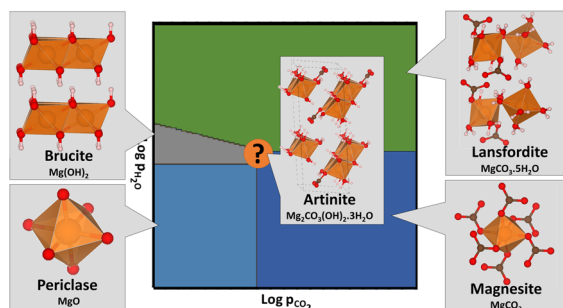
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Effect of frequency on the classical and relaxor ferroelectric behavior of substituted titanate $\text{Ba}_{0.7}\text{Er}_{0.16}\text{Ca}_{0.05}\text{Ti}_{0.91}\text{Sn}_{0.09}\text{O}_3$

A. Saidi,* A. Mabrouki, J. Dhahri, E. Dhahri, K. Khirouni and B. F. O. Costa

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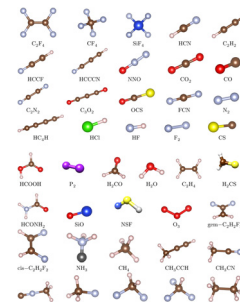


Location of Artinite ($\text{Mg}_2\text{CO}_3(\text{OH})_2 \cdot 3\text{H}_2\text{O}$) within the $\text{MgO}-\text{CO}_2-\text{H}_2\text{O}$ system using *ab initio* thermodynamics

Joshua S. Tse, James Grant, Jonathan M. Skelton, Lisa J. Gillie,* Runliang Zhu, Giovanni L. Pesce, Richard J. Ball, Stephen C. Parker* and Marco Molinari*

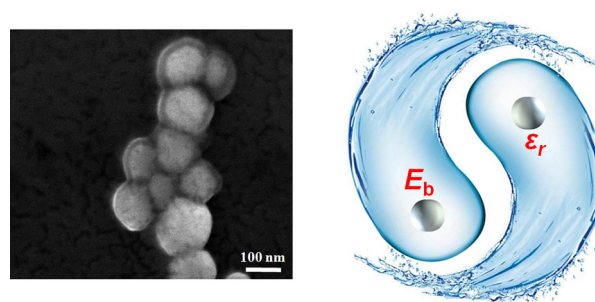


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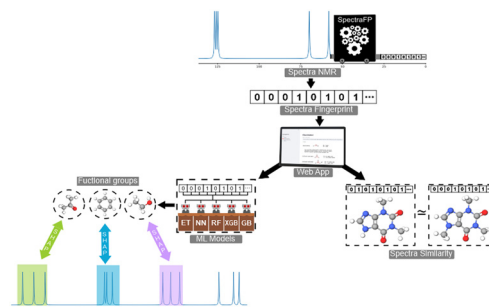
Optimizing the dielectric constant of the shell layer in core-shell structures for enhanced energy density of polymer nanocomposites

Quan-Ping Zhang,* Fang-Yan Du, Xiu Liu, Jia-Hao Lv,
Li He, Jia-Le Li, Yin-Tao Li and Yuan-Lin Zhou



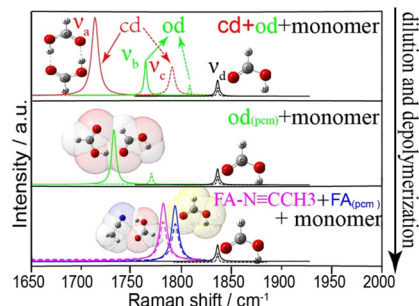
SpectraFP: a new spectra-based descriptor to aid in cheminformatics, molecular characterization and search algorithm applications

Jefferson R. Dias-Silva,* Vitor M. Oliveira,
Flávio O. Sanches-Neto, Renan Z. Wilhelms and
Luiz H. K. Queiroz Júnior*



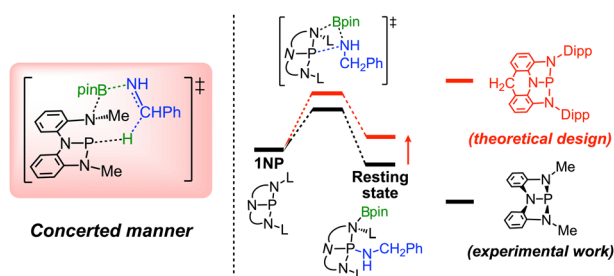
Study on depolymerization kinetics of formic acid dimers in binary mixture

Yufei Han, Zian Wang, Ru Qiao, Jianwen Cheng,
Caiying Jiang* and Huigang Wang*



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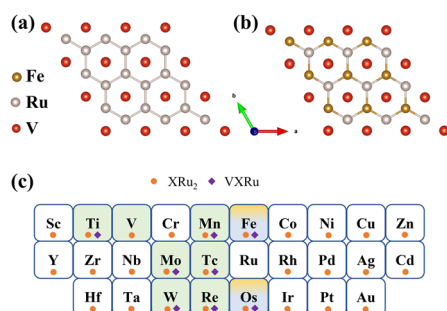
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Metal-free catalytic hydroboration of imine with pinacolborane using a pincer-type phosphorus compound: mechanistic insight and improvement of the reaction

Deshuai Yang, Shuoqi Zhang, Guixiang Zeng* and Zhao-Xu Chen*

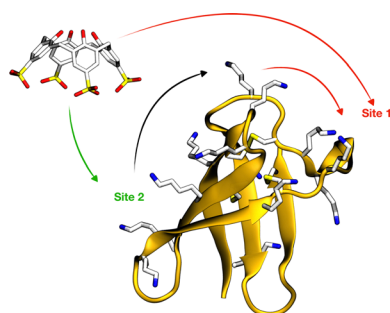
18062



Versatile transition metal monolayers with catalytic and superconducting properties: a computational study

Xue Li, Hanyu Liu* and Siyu Lu*

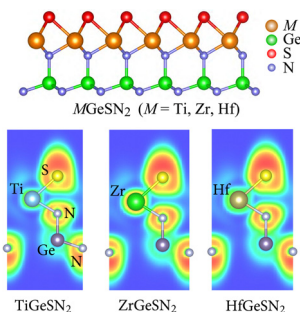
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Probing the dynamical interaction of the *para*-sulfonato-calix[4]arene with an antifungal protein

Alessio Bartocci* and Elise Dumont

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Strain-induced phase transitions and high carrier mobility in two-dimensional Janus MGeSN₂ (M = Ti, Zr, and Hf) structures: first-principles calculations

Le C. Nhan, Nguyen T. Hiep, Cuong Q. Nguyen and Nguyen N. Hieu*

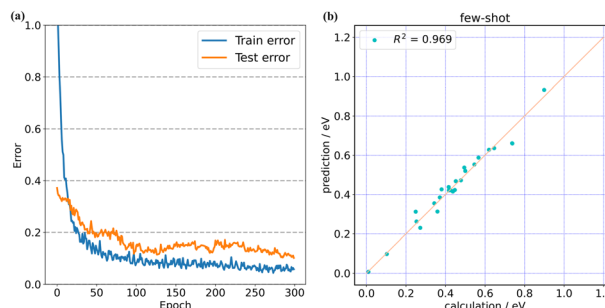


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Machine learning-aided band gap prediction of semiconductors with low concentration doping

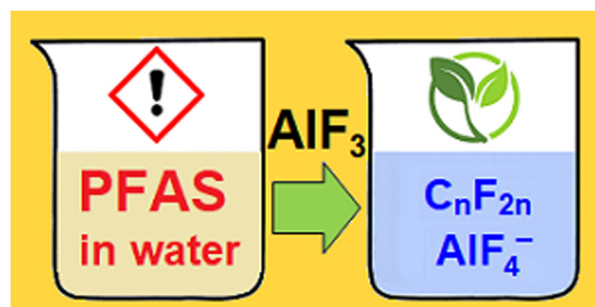
Yuqi Tang, Haiyuan Chen, Jianwei Wang* and Xiaobin Niu*



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Degradation of selected perfluoroalkyl substances (PFASs) using AlF_3 in water

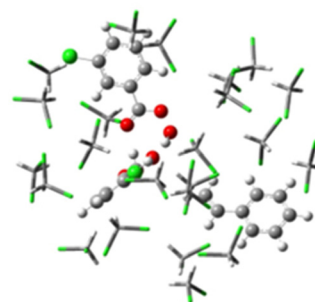
Marcin Czaplak* and Piotr Skurski*



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Theoretical and experimental mechanistic study of water molecule involvement in the Prilezhaev reaction

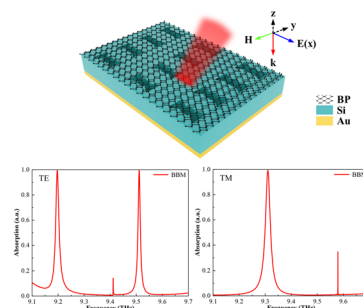
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18109

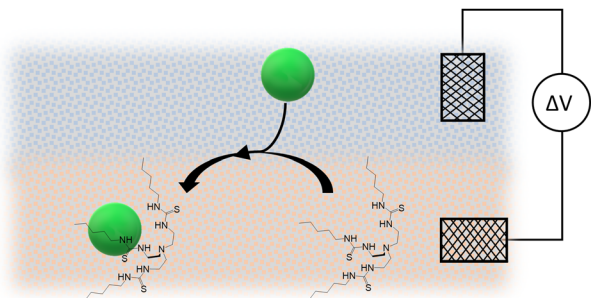
A tunable perfect absorber based on a black phosphorus/bowtie shaped cavity hybrid metasurface

Boxun Li,* Yi Wei, Lili Zeng,* Mingliang Liu, Ruquan Wen, Xingjiao Zhang and Chaosheng Deng



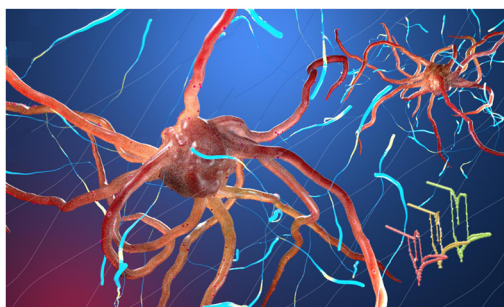
RESEARCH PAPERS

18121

**Electrochemical assessment of a tripodal thiourea-based anion receptor at the liquid|liquid interface**

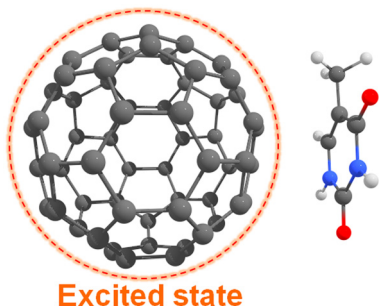
Hussain A. Al Nasser, Luis Martinez-Crespo, Simon J. Webb and Robert A. W. Dryfe*

18132

**Forming-free plant resistive random access memory based on the Coulomb blockade effect produced by gold nanoparticles**

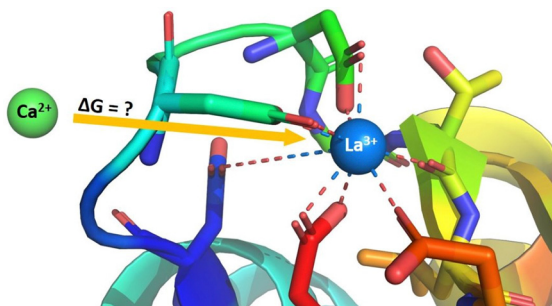
Lu Wang,* Jiachu Xie and Dianzhong Wen

18139

**Energy decomposition analysis methods for intermolecular interactions with excited states**

Zhen Tang, Boxiao Shao, Wei Wu and Peifeng Su*

18149

**Electrostatic interactions – key determinants of the metal selectivity in La³⁺ and Ca²⁺ binding proteins**

Silvia Angelova,* Nikoleta Kircheva, Valya Nikolova, Stefan Dobrev and Todor Dudev*

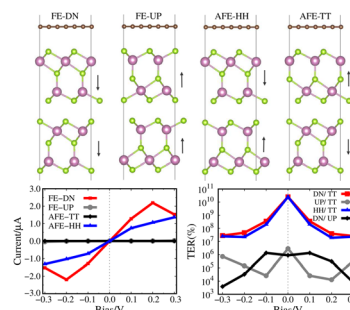


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18158

Giant tunneling electroresistance in a 2D bilayer-In₂Se₃-based out-of-plane ferroelectric tunnel junction

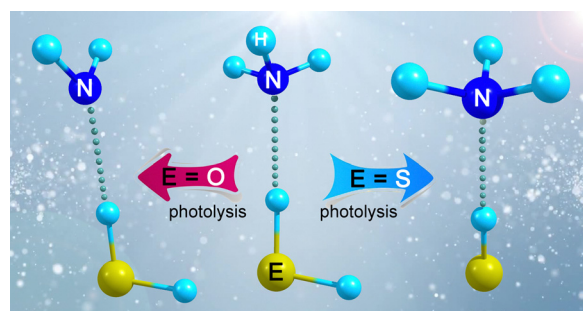
Ziqi Han, Chun-Sheng Liu, Xiaohong Zheng* and Lei Zhang*



18166

Spectroscopic identification of the ammonia–mercapto radical complex

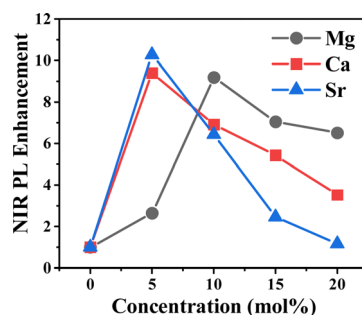
Junfei Xue, Xin Shao, Xin Jiang and Xiaoqing Zeng*



18175

Alkaline earth metal ion doping to enhance the light emission from Er³⁺:SnO₂ nanocrystal Co-doped silica films

Enze Qu, Yangyi Zhang, Lixiang Wang, Jiaming Chen, Dongke Li, Jingjie Zhao, Jun Xu* and Kunji Chen

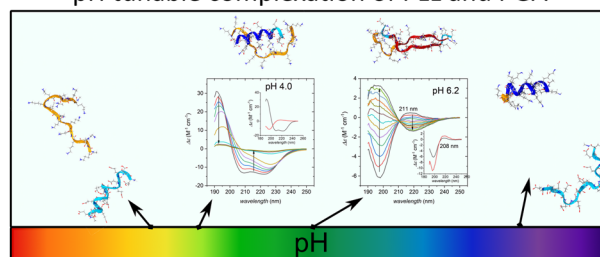


18182

pH dependence of the assembly mechanism and properties of poly(L-lysine) and poly(L-glutamic acid) complexes

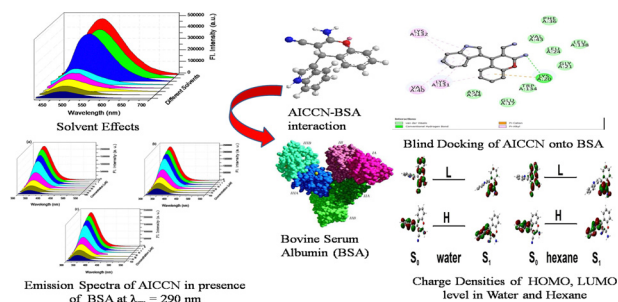
Tuuva Kastinen, Dawid Lupa, Piotr Bonarek, Dmitrii Fedorov, Maria Morga, Markus B. Linder, Jodie L. Lutkenhaus, Piotr Batys* and Maria Sammalkorpi*

pH tunable complexation of PLL and PGA



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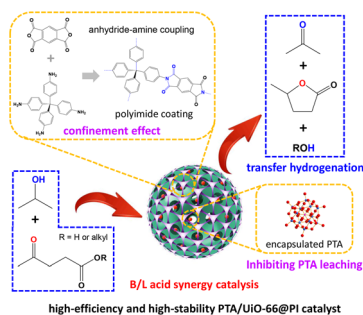
18197



Fluorescence probing and molecular docking analysis of the binding interaction of bovine serum albumin (BSA) with the polarity probe AICCN

Barun Mandal, Nilkanta Chowdhury, Nabajyoti Baildya, Ranju Prasad Mandal, Angshuman Bagchi and Swati De*

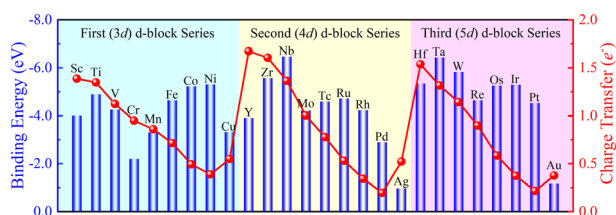
18215



Surface-sealing encapsulation of phosphotungstic acid in microporous UiO-66 as a bifunctional catalyst for transfer hydrogenation of levulinic acid to γ -valerolactone

Hongzi Tan, Siteng Rong, Zhiyuan Zong, Pengrui Zhang, Rongrong Zhao, Feng Song, Hongyou Cui,* Zhe-Ning Chen,* Weiming Yi and Fengshan Zhang*

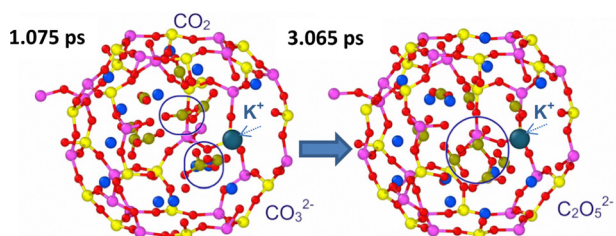
18224



Theoretical screening of a graphyne-supported transition metal single-atom catalyst for the N_2 reduction reaction

Min Li, Qinglong Fang,* Xumei Zhao,* Caijuan Xia, Anxiang Wang, You Xie, Fei Ma, Jianmei She and Zhongxun Deng

18233



A forgotten participant in pore deblocking of zeolites: dicarbonate in NaMeA zeolites, Me = Na, K, Rb, Cs

Ilya A. Bryukhanov, Andrey A. Rybakov and Alexander V. Larin*

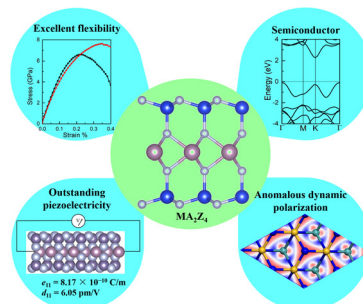


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18247

Flexible MA_2Z_4 ($\text{M} = \text{Mo}, \text{W}$; $\text{A} = \text{Si}, \text{Ge}$ and $\text{Z} = \text{N}, \text{P}, \text{As}$) monolayers with outstanding mechanical, dynamical, electronic, and piezoelectric properties and anomalous dynamic polarization

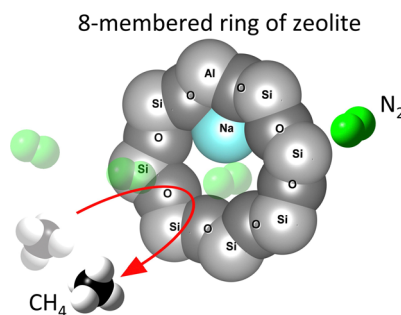
Xinxin Wang,* Weiwei Ju, Dandan Wang, Xiaohong Li and Jianguo Wan



18259

Nitrogen rejection in natural gas using NaZSM-25 zeolite

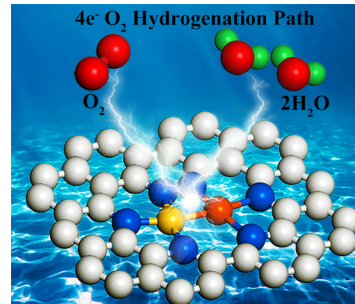
Seyed Hesam Mousavi, Javad Tamnanloo, Abdol Hadi Mokarizadeh, Ali Zavabeti, Jefferson Zhe Liu* and Gang Kevin Li*



18266

NiPd co-doped nitrogen-coordinated graphene as a high-efficiency electrocatalyst for oxygen reduction reactions: a first-principles determination

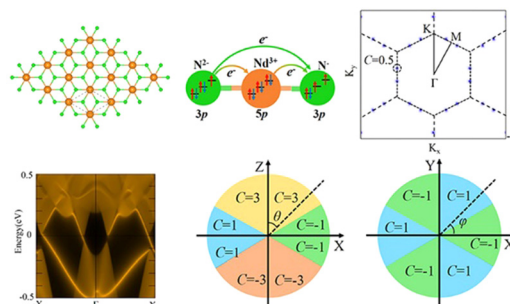
Kaiwen Huang, Weihua Yang, Lei Li,* Yameng Li, Rao Huang and Yuhua Wen*



18275

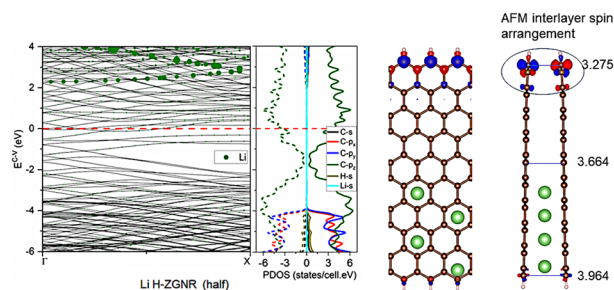
Quantum anomalous Hall effect with a high and tunable Chern number in monolayer NdN_2

Shengshi Li, Xinyang Li, Weixiao Ji,* Ping Li, Shishen Yan and Changwen Zhang*



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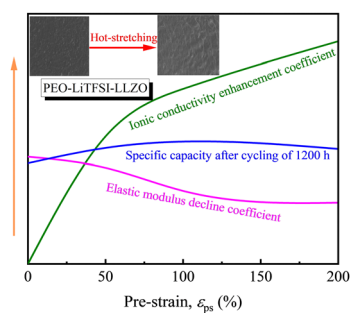
18284



Fundamental properties of alkali-intercalated bilayer graphene nanoribbons

Thi My Duyen Huynh, Guo-Song Hung, Godfrey Gumbs and Ngoc Thanh Thuy Tran*

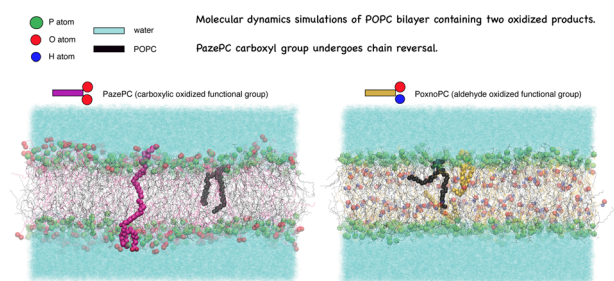
18297



Enhancing the ionic conductivity and mechanical properties of PEO-based solid electrolytes through thermal pre-stretching treatment

Lifa Zhang, Liang Fu, Weisi Qin, Yaolong He, Hong Liu* and Hongjiu Hu*

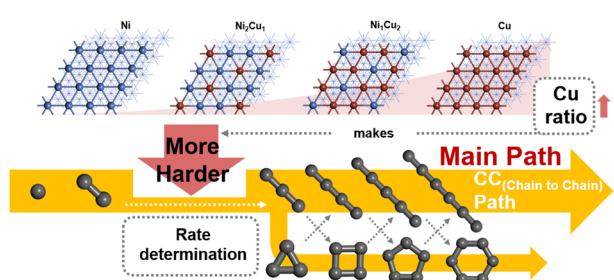
18310



Effect of oxidation on POPC lipid bilayers: anionic carboxyl group plays a major role

Behnaz Bagheri,* Phansiri Boonnoy, Jirasak Wong-ekkabut and Mikko Karttunen

18322



Effects of Cu ratios on the C₁–C₆ growth mechanism on copper–nickel bimetallic surfaces

Cunxin Zhang, Juntian Niu,* Zeyu Guo, Haiyu Liu, Yan Jin and Jingyu Ran

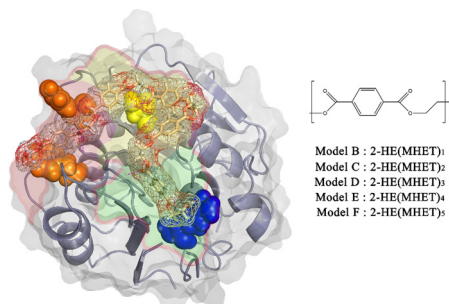


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18332

Atomistic insight into the binding mode and self-regulation mechanism of *Is*PETase towards PET substrates with different polymerization degrees

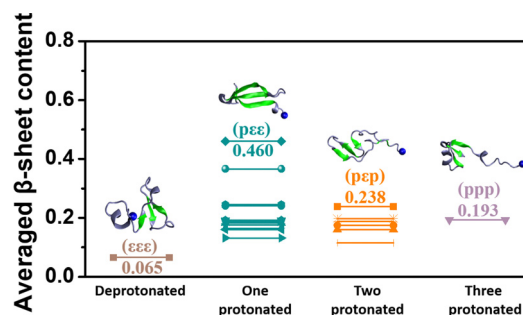
Linyu Chen, Fangfang Fan,* Meiyuan Yang, Linqun Wang, Yushuo Bai, Shuai Qiu, Changjiang Lyu and Jun Huang*



18346

The effect of histidine behaviors on the structural properties of Aβ(1–42) peptide in protonation stage one, two, and three

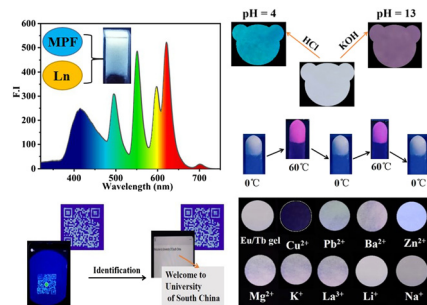
Yue Sun, Changgui Li, Jinping Wang* and Hu Shi*



18354

White-light-emitting Ln-hydrogels with multi-stimuli responsiveness and applications in environmental sensing and anti-counterfeiting

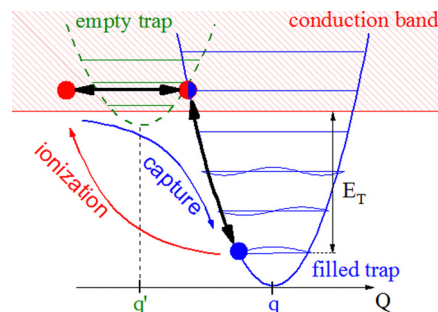
Xiao-Juan Wang, Hong-Lin Mo, Chuan-Wan Wei,* Shu-Qin Gao and Ying-Wu Lin*



18364

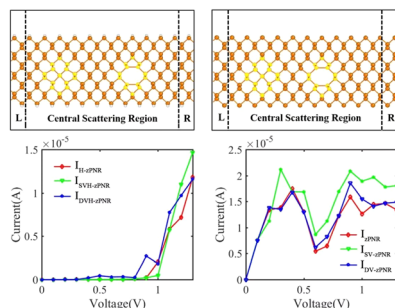
A quantum model of charge capture and release onto/from deep traps

Ivan I. Vrubeľ,* Vasilii Khanin, Markus Suta, Roman G. Polozkov and Evgeniia D. Cherotchenko



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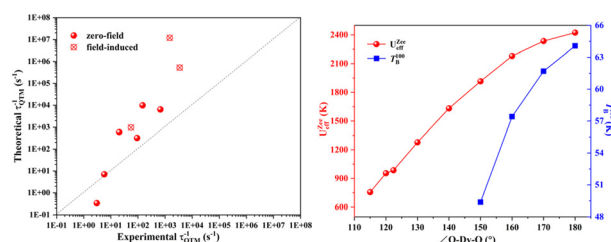
18378



Effect of vacancy defects on transport in all-phosphorene nanoribbon devices from first principles

Jingyuan Huang, Qiang Zhang,* Xiaojie Liu,* Yin Wang* and Haitao Yin*

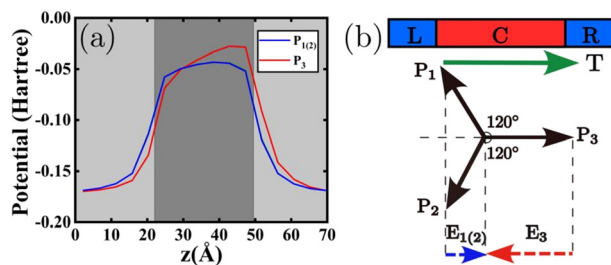
18387



Ab initio prediction of key parameters and magneto-structural correlation of tetracoordinated lanthanide single-ion magnets

Qi-Qi Yang, Yu-Fei Wang, Yu-Xi Wang, Ming-Jing Tang and Bing Yin*

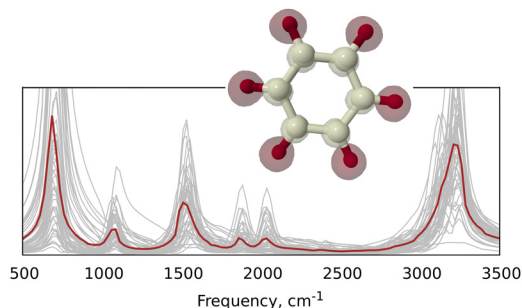
18400



Tunnel electroresistance effect in a two-dimensional organic ferroelectric tunnel junction

Huizhen Han, Xiaoli Zhang, Lili Kang,* Xiaohong Zheng* and Gaofeng Zhao*

18406



Describing nuclear quantum effects in vibrational properties using molecular dynamics with Wigner sampling

Denis S. Tikhonov* and Yury V. Vishnevskiy*

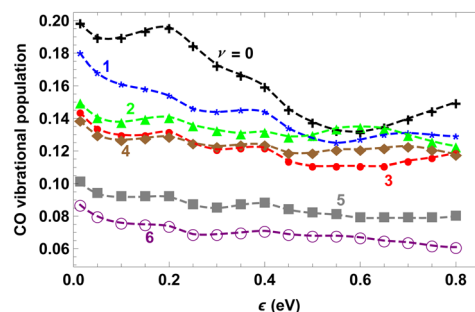


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18424

Direct dissociative recombination of HCO^+ via the core-excited doublet and the lowest quartet states

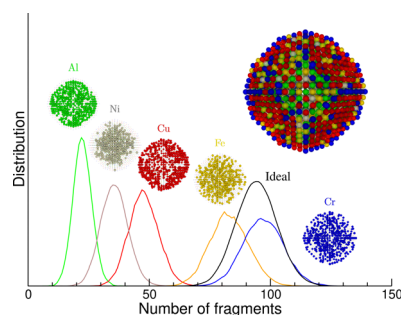
Martin Lehner and Martin Jungen*



18439

The interplay between size, shape, and surface segregation in high-entropy nanoalloys

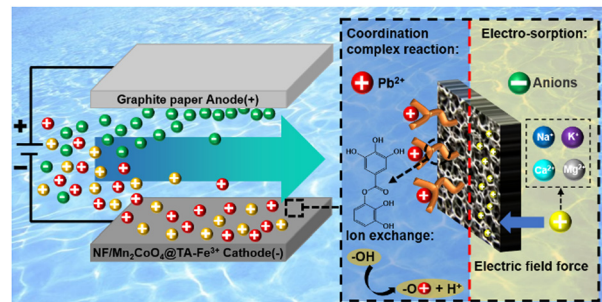
Florent Calvo



18454

Selective capacitive removal of Pb^{2+} ion contaminants from drinking water via nickel foam/ Mn_2CoO_4 @tannic acid- Fe^{3+} electrodes

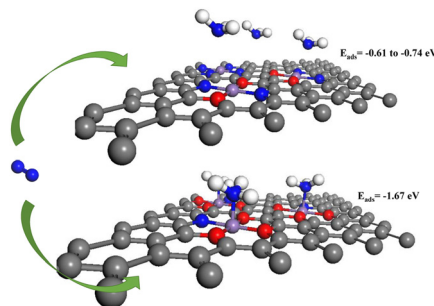
Changbin Tang,* Yongqi Yu, Yuzhu Shi, Yanrong Li, Yujie Zhang and Juanqin Xue



18465

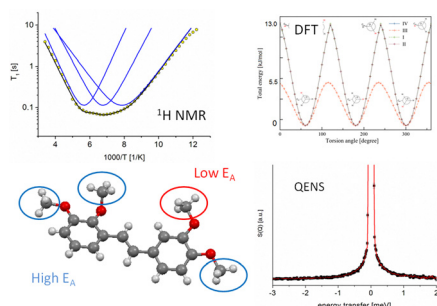
Adsorption mechanism of the N_2 and NRR intermediates on oxygen modified MnN_4 -graphene layers – a single atom catalysis perspective

A. E. Genç* and I. C. Tranca



RESEARCH PAPERS

18481



Experimental and theoretical insights into the structure and molecular dynamics of 2,3,3',4'-tetramethoxy-*trans*-stilbene – a chemopreventive agent

Aleksandra Pajzderska,* Marcin Wierchowski, Dawid Łażewski, Agnieszka Gielara-Korzańska, Artur Korzański, Łukasz Popenda, Jacek Jencyk, Fanni Juranyi, Jan P. Embs and Jan Wąsicki

CORRECTIONS

18495

Correction: Delivery mechanism of doxorubicin by PEG–DPPE micelles on membrane invasion by dynamic simulations

Lina Zhao, Meina Ren, Yanjiao Wang, Hailong An* and Fude Sun*

18496

Correction: Sizable magnetic entropy change in bismuth-substituted $\text{La}_{0.75}\text{Bi}_{0.1}\text{Na}_{0.15}\text{MnO}_3$ manganite

Lozil Denzil Mendonca, M. S. Murari and Mamatha D Daivajna*

18497

Correction: Comparative study on formic acid sensing properties of flame-made Zn_2SnO_4 nanoparticles and its parent metal oxides

Matawee Pungsang, Kanittha Inyawilert, Mameaseng Siriwalai, Anurat Wisitsoraat, Adisorn Tuantranont and Chaikarn Liewhiran*

