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Cover

See Xue-Bin Wang, Zhenrong Sun, Yan Yang *et al.*, pp. 12657–12665. Image reproduced by permission of Yan Yang from *Phys. Chem. Chem. Phys.*, 2025, 27, 12657.



Inside cover

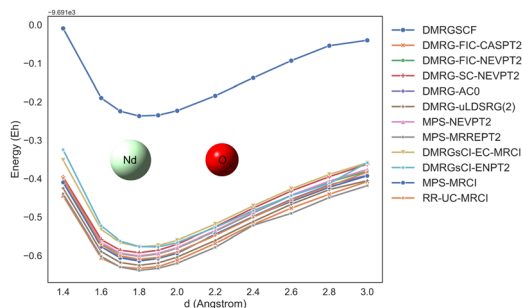
See Cercis Morera-Boado, Tina A. Harriott, Daniel Majaess, Chérif F. Matta *et al.*, pp. 12666–12674. Image reproduced by permission of Chérif F. Matta from *Phys. Chem. Chem. Phys.*, 2025, 27, 12666. Plot generated using data from Haoyu Fan *et al.*, 2019, *ApJ*, 878, 151

PERSPECTIVES

12622

Describing dynamic electron correlation beyond a large active space

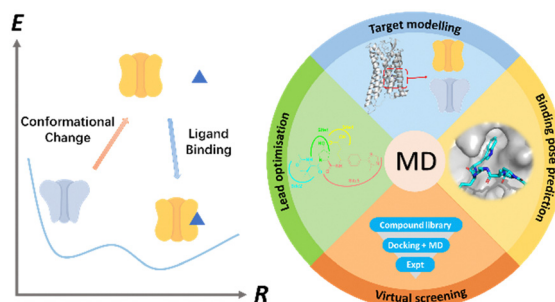
Yinxuan Song, Yifan Cheng* and Haibo Ma*



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Molecular dynamics-driven drug discovery

Dengjie Yan, Yue Ma, Xiang Chen, Shi Deng and Qiantao Wang*



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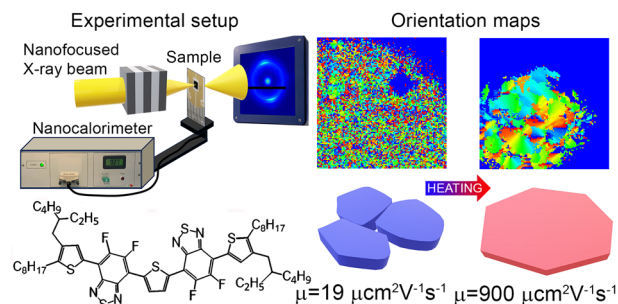


COMMUNICATION

12652

Correlation between domain size and charge transport properties in benzothiadiazole–thiophene molecules: insights from nano-focus X-ray scattering and fast scanning chip calorimetry

Azaliia F. Akhiamova, Ainur F. Abukaev, Mariia V. Gaikovich, Ilya E. Kuznetsov, Alexey A. Piryazev, Ilya I. Rulev, Alexander V. Akkuratov, Denis V. Anokhin and Dimitri A. Ivanov*

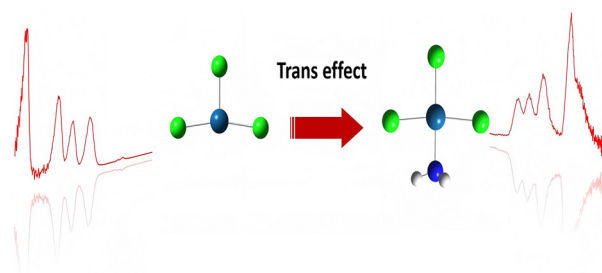


RESEARCH PAPERS

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Exploring the *trans* effect of the NH_3 ligand in platinum halide complexes $\text{Pt}(\text{NH}_3)\text{ClX}_2^-$ ($\text{X} = \text{Cl}, \text{Br}, \text{I}$) using cryogenic photoelectron spectroscopy and quantum chemical calculations

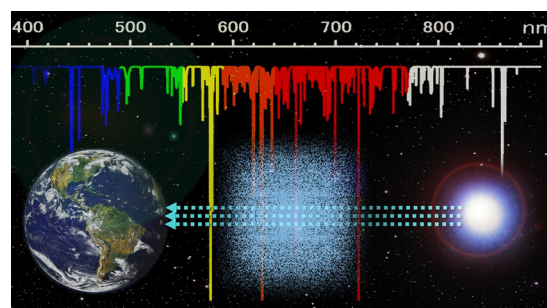
Qixu Zhao, Jian Zhang, Xueying Li, Peng Tang, Fan Yang, Junyang Ma, Zhubin Hu, Haitao Sun, Xue-Bin Wang,* Zhenrong Sun* and Yan Yang*



12666

Vetting molecular candidates posited for the first diffuse interstellar bands (5780 and 5797 Å): a quantum chemical study

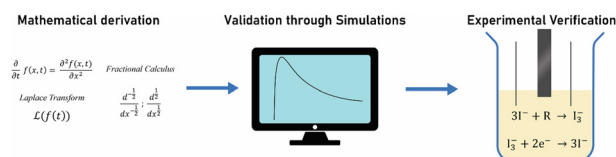
Halis Seuret, Ailish D. Sullivan, Cercis Morera-Boado,* Tina A. Harriott,* Daniel Majaess,* Lou Massa and Chérif F. Matta*



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A new approach to a first order irreversible homogeneous chemical reaction followed by an electrochemical process (C_iE mechanism): theory, simulation and application

Rafael A. L. Chioquetti, Raphael P. Bacil and Silvia H. P. Serrano*



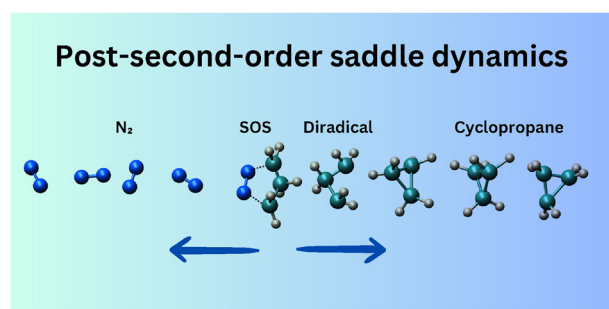
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VaporFit: an open-source software for accurate atmospheric correction of FTIR spectra

Przemysław Pastwa and Piotr Bruździak*

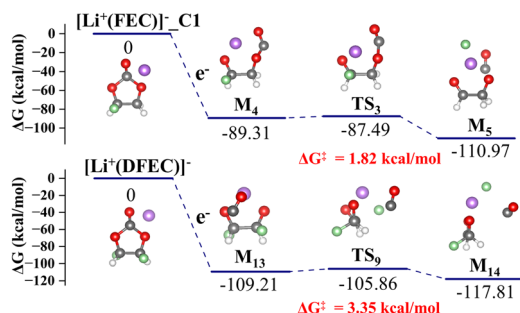
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Dynamical insights into denitrogenation of 1-pyrazoline: exploring pathways *via* transition states and a second-order saddle

Renuka Pradhan and Upakarasamy Lourderaj*

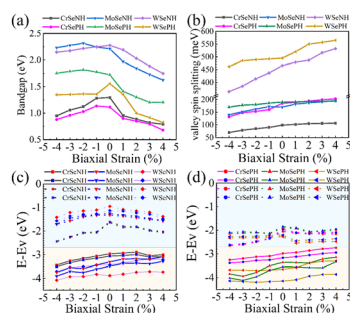
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Mechanistic insights into the thermodynamics and kinetics underlying the reductive decomposition of fluoroethylene and difluoroethylene carbonates for SEI formation in LIBs

Ruru Song, Tairan Wang, Yiyang Pan, Cuili Zhang, Lang Wang, Shengbo Lu, Tracy Chenmin Liu, Shihan Qi, Weiguo Huang, Jingjing Liu, Guannan Zhu* and Jun Fan*

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Strong spin-orbit coupling effect induced large valley splitting in Janus MSeXH (M = Cr, Mo, and W; X = N and P)

Yang Zhang, Shi-qian Qiao, Cheng-long Wu, Zhi-qiang Ji, Hong Wu and Feng Li*

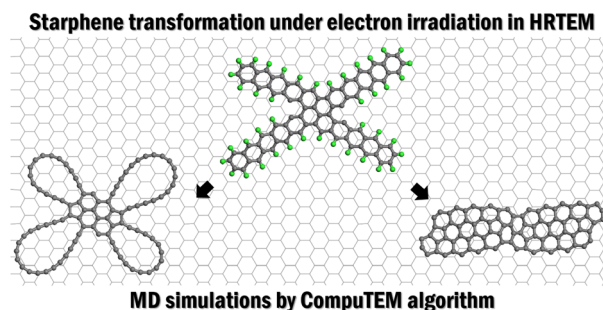


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Transformation of starphenes into amorphous graphene nanoribbons with attached carbon chains under electron irradiation

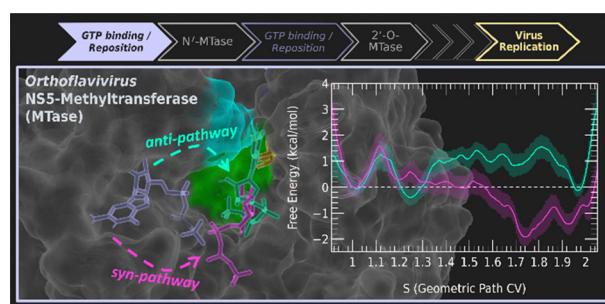
Alexander S. Sinitsa,* Yulia G. Polynskaya, Yegor M. Kedalo, Andrey A. Knizhnik and Andrey M. Popov



12738

Reposition pathways of GTP in *orthoflavivirus* NS5-methyltransferase revealed by enhanced molecular dynamics simulations

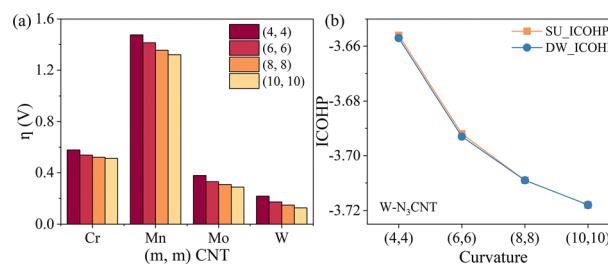
Lok Wan Ng, Yuen-Kit Cheng, Wei Shen Aik* and Wei Han*



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First-principles and machine learning study of the NRR in curvature-tuned TM-doped CNTs

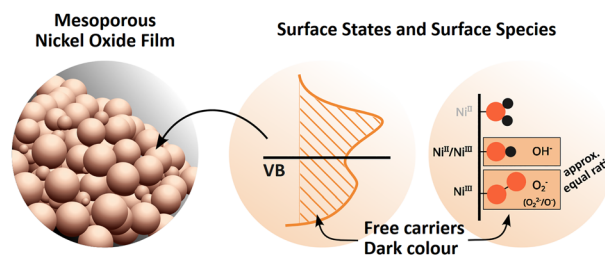
Xiaolin Jiang, Hongchang Xu, Lifu Zhang and Zhenpeng Hu*



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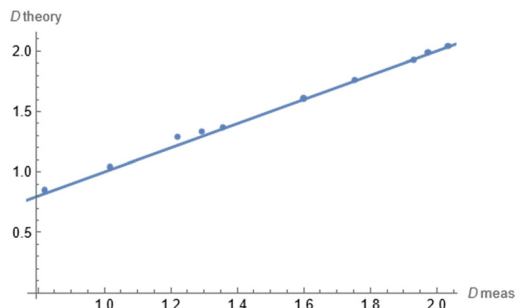
Insights into the surface of mesoporous nickel oxide and its interaction with oxygen and water

Sina Wrede, Qianhui Liu, Libo Chen, Luca D'Amario, Bin Cai, Mattia Scardamaglia, Zhi-Bin Zhang, Maria Hahlin* and Haining Tian*



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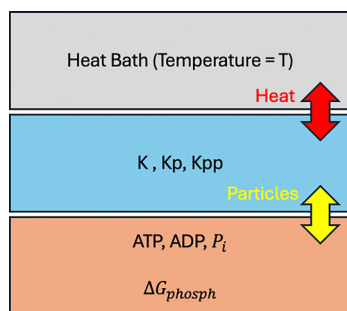
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The Poisson equation and polarization charge density in the concentration gradient of a diffusing electrolyte

Gerald S. Manning

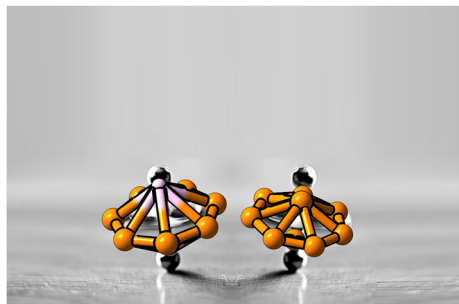
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Fluctuating signal and reversibility limit information and entropy in a MAPK signalling cascade

Harshita Saxena and Rati Sharma*

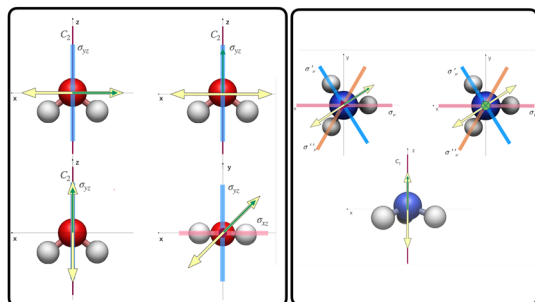
12793



Al₂B₇: an extension of the inverse sandwich B₉ cluster featuring Lewis acid sites and planar aromaticity

Peter L. Rodríguez-Kessler* and Alvaro Muñoz-Castro*

12801

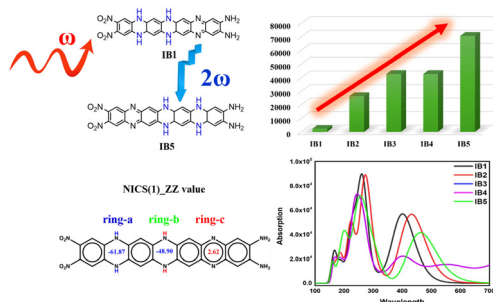


Dynamical symmetries and selection rules in high-harmonic generation spectroscopy of nonlinear molecules

Marco Marchetta, Eleonora Luppi* and Emanuele Coccia*



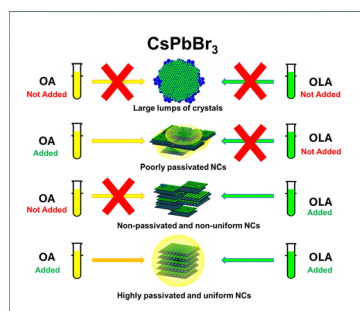
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Exploring the role of H-migration in the aromaticity, spectroscopic, photovoltaic and optical properties of planar heterocyclic compounds: a DFT study

Muhammad Ibrahim, Farah Tayyaba Khan, Hong-Liang Xu* and Muhammad Arif Ali*

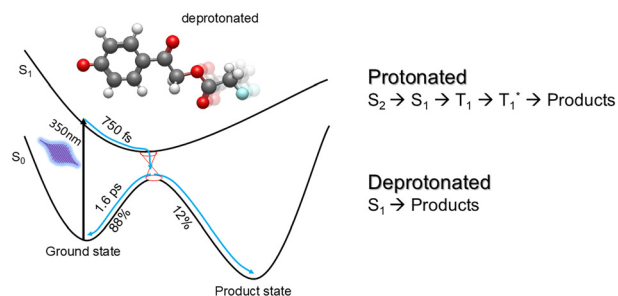
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Striking the balance between the capping ligands for CsPbBr₃ nanocrystal synthesis *via* an emulsion LARP approach

Govind B. Nair,* Sumedha Tamboli, Sanjay J. Dhoble and Hendrik C. Swart*

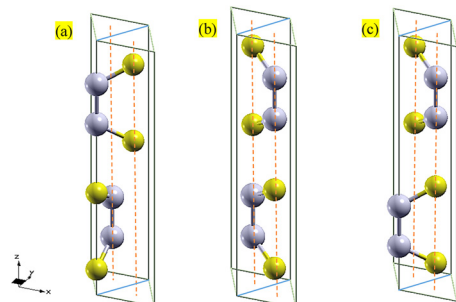
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pH-dependent ultrafast photodynamics of *p*-hydroxyphenacyl: deprotonation accelerates the photo-uncaging reaction

Yannik Pfeifer, Till Stensitzki, Jakub Dostál, Evgenii Titov, Miroslav Kloz, Peter Saalfrank and Henrike M. Müller-Werkmeister*

12908



Layer-dependent electronic, vibrational and optical properties of 2D AISe crystals

Mousa Bejani,* Olivia Pulci, Naser Karimi and Friedhelm Bechstedt

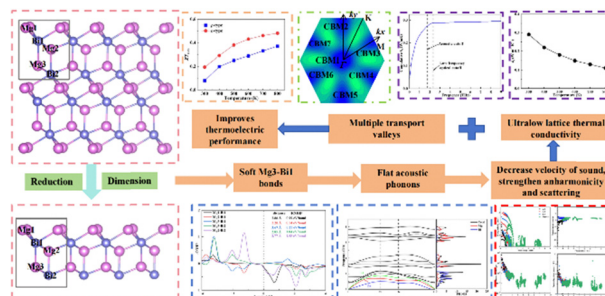


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Unraveling the lattice thermal conductivity and thermoelectric properties of monolayer Mg_3Bi_2

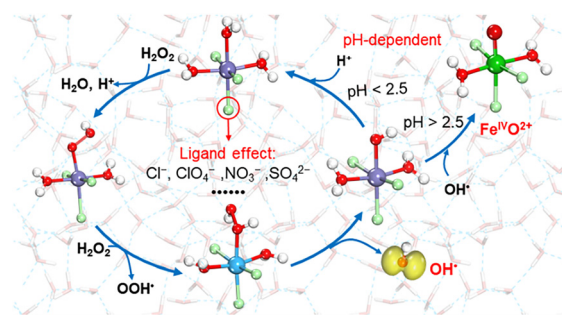
Yingying Chen, Zheng Ma, Na Zhao, Yajun Li, Xi Yao and Xilong Dou*



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Computationally revisiting pH- and ligand-dependence of Fenton reaction selectivity and activity in aqueous solution

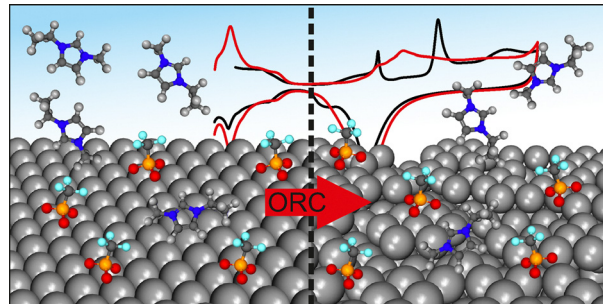
Ying Liu, Peijun Hu and Haifeng Wang*



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How the ionic liquid $[\text{C}_2\text{C}_1\text{Im}][\text{OTf}]$ affects the stability of Pt(111) during potential cycling

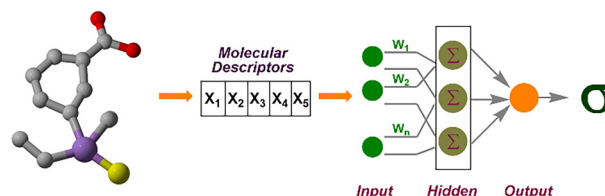
Felix Hilpert, Yunsheng Qiu, Leopold Lahn, Kevin Höllring, Nicola Taccardi, Peter Wasserscheid, Olga Kasian, Ana-Sunčana Smith, Karl J. J. Mayrhofer, Valentin Briega-Martos, Serhiy Cherevko, Olaf Brummel* and Jörg Libuda



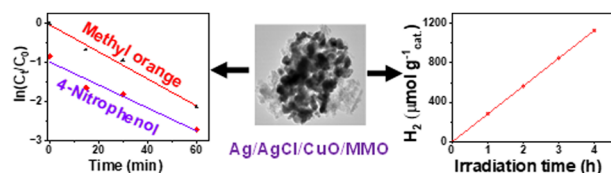
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A machine learning-driven prediction of Hammett constants using quantum chemical and structural descriptors

Vaneet Saini* and Ranjeet Kumar



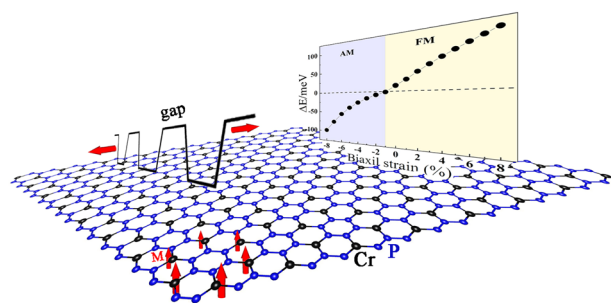
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Hierarchical microspheres of a mixed metal oxide heterojunction with CuO and Ag/AgCl for enhanced photocatalytic oxidation of organic pollutants and hydrogen production

Manish Verma, Neha Verma, Swaraj Servottam, Ramya Prabhu B and Neena S. John*

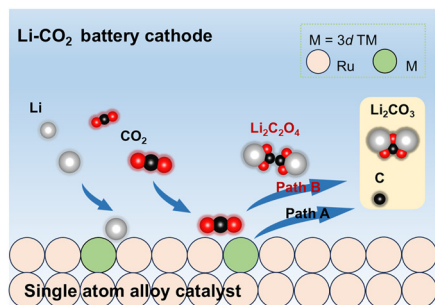
12979



Magnetic switching and quantization of bandgap in 2D graphene-like CrP_3

Hong-yao Liu, Mi He, Huan Yang* and Yujun Zheng*

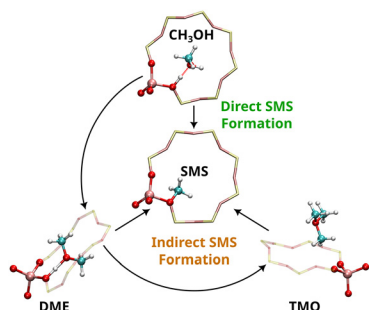
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Promising Ru-based cathode catalysts for Li- CO_2 batteries via single-atom alloying

Jinhui Zhang, Yao Liu, Tengwen Yan, Guanghui Jin, Jianru Zhao, Yuxuan Wang, Dashuai Wang* and Jing Xu*

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A computational study of the formation of surface methoxy species in H-SSZ-13 and H-SAPO-34 frameworks

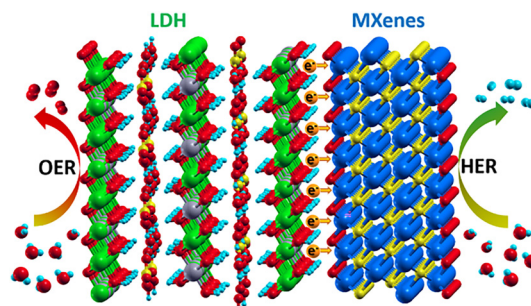
Gabriel Bramley, Oscar van Vuren and Andrew J. Logsdail*



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MXenes enhance electrocatalytic water electrolysis of NiFe layered double hydroxides through bifunctional heterostructuring

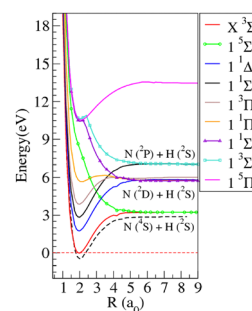
Nannan Li, Xiaotong Han, Ho Seok Park and Jin Yong Lee*



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Rydberg states and new resonant states of the imidogen molecule NH: pathways for nitrogen release

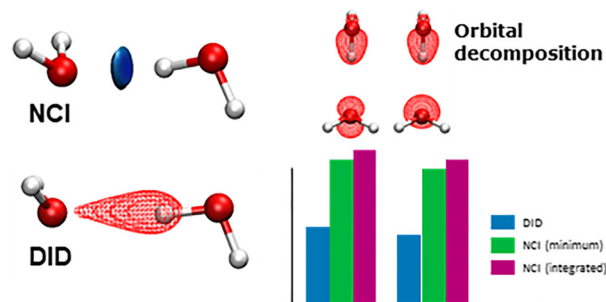
Raju Ghosh, Binayak Samaddar Choudhury, János Zsolt Mezei, Ioan F. Schneider, Nicolina Pop and Kalyan Chakrabarti*



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NCI orbital decomposition and critical comparison to local correlation schemes

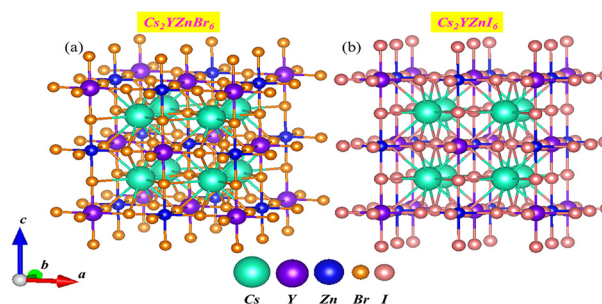
Xaiza Aniban, Maxime Ferrer, M. Merced Montero-Campillo, Ricardo A. Mata,* Julia Contreras-García* and Martí Gimferrer*



13043

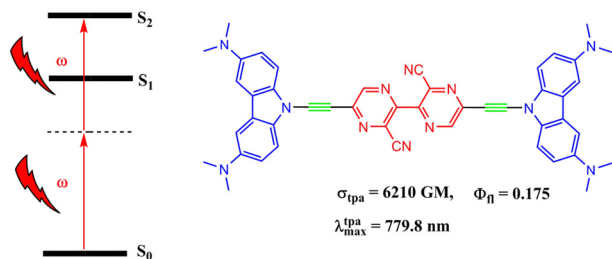
First principles insight into Cs₂YZnX₆ (X = Br, I) double perovskite materials for optoelectronic and thermoelectric device applications

Abid Zaman,* Salhah Hamed Alrefaee, Muawya Elhadi, Pervaiz Ahmad, Mukhlisa Soliyeva, Naseem Akhter, Nouredine Elboughdiri, Vineet Tirth, Ali Algahtani, Amnah Mohammed Alsuhailani and Moamen S. Refat



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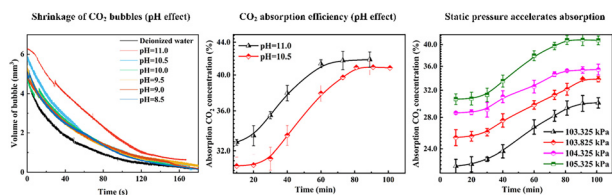
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Theoretical study of the two-photon absorption and fluorescence emission properties of bipyrazine (or hexaazatriphenylene) core based donor- π -acceptor- π -donor framework chromophores

Chunyun Tu,* Weijiang Huang, Sheng Liang, Kui Wang and Yi Guo

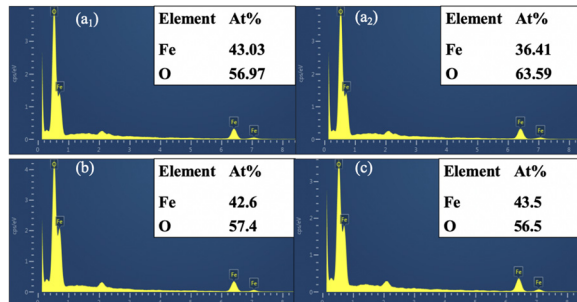
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Study on the mass transfer behavior of single CO₂ bubbles in sodium silicate solution

Guangyan Hu, Ruoxi Zhang, Xiaomei Tang, Pengyue Sun* and Taiyu Wang*

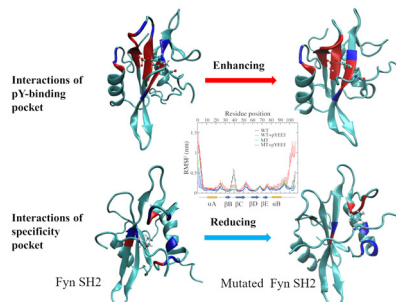
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Preparation of non-spherical nano-Fe₃O₄ and its effect on thermal decomposition of AP and combustion performance of composite fuels

Ruiling Xie, Hongyang Li,* Hong Li, Shentao Zeng, Lixiaosong Du,* Qing Cai, Sujun Shi, Wenqi Xu, Ran Wang, Cui Luo and Ying Liu

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Mutation-induced rigidity in the Fyn SH2 domain enhances pY-binding affinity at the cost of peptide specificity

Li Deng, Yang Zou, Junbao Zhu, Lei Li* and Yanting Wang*

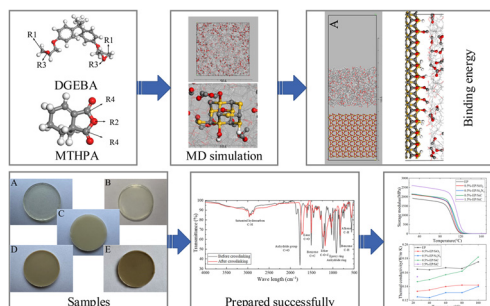


RESEARCH PAPERS

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A study on the thermodynamic performance of nano-silicide filled epoxy resin composite materials

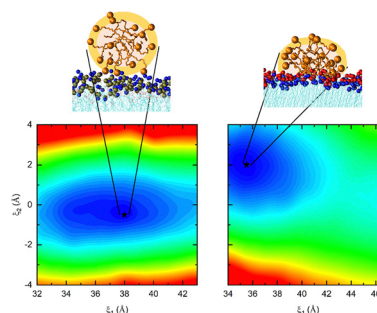
Hang Zhang, Zhijin Zhang,* Chao Liu, Xingliang Jiang, Jianlin Hu and Qin Hu



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Influence of lipid bilayer head group polarity on micelle behavior and surfactant transfer: a molecular dynamics simulation study

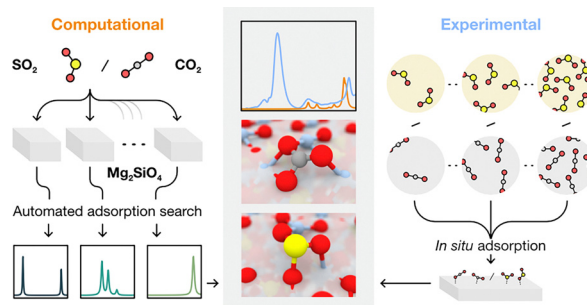
Yeonho Song and Hyonseok Hwang*



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Revealing SO₂ and CO₂ adsorption features on forsterite via IR spectroscopy and automated computational approaches

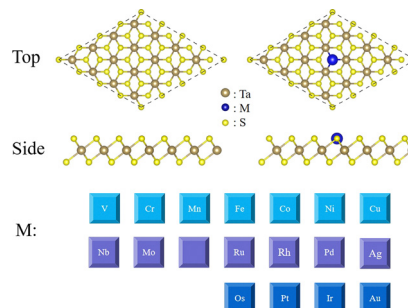
Eric Mates-Torres,* Guillermo Escolano Casado, Lorenzo Mino,* Nadia Balucani, Piero Ugliengo and Albert Rimola*



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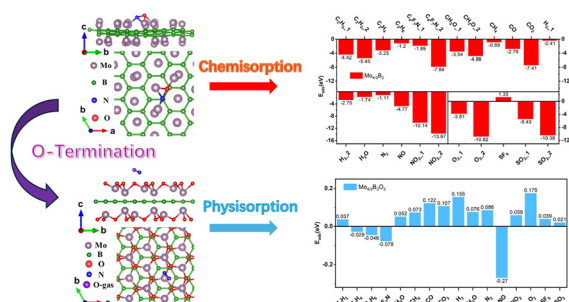
Computational screening of transition-metal atom embedding in 1T-TaS₂ monolayer defects as efficient oxygen-reduction/evolution-reaction bifunctional catalysts

Junkai Xu, Rongxing Zhang, Yu Wu, Tongmeng Xing, Jianjun Fang,* Jing Li,* Xianfang Yue* and A. J. C. Varandas*



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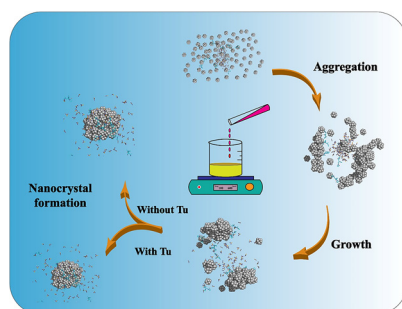
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Achieving tunable adsorption selectivity and sensitivity of boridenes for gas detection by surface O-termination engineering

Sateng Li, Haoliang Liu, Yuxuan Hou, Qin Jiang, Kai Wu, Yonghong Cheng and Bing Xiao*

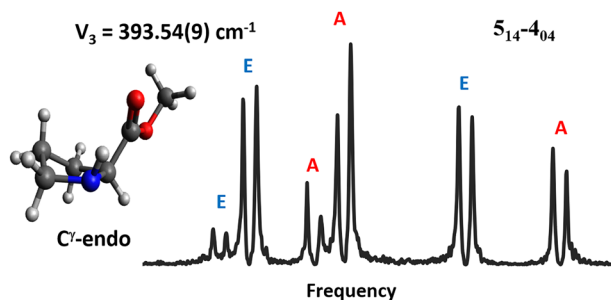
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Mechanistic insights on sulfur functionalization of Ag nanoflowers

Arup K. De, Ravishankar Srivastava, Nirupam Das, Partho Sarathi Gooh Pattader* and Rajiv K. Kar*

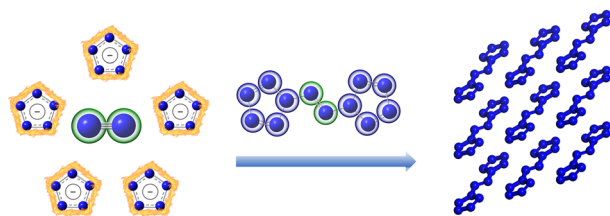
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The challenging conformer assignment of proline methyl ester from rotational spectroscopy

Dinesh Marasinghe, Michael J. Carrillo, Dakota Z. Smallridge, Kaitlyn E. Butts, Bijaya Bagale and Michael J. Tubergen*

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Theoretical prediction of pressure-stabilized all-nitrogen N₁₂ molecular crystals with π - π stacking

Lei Zhao,* Zelin Ma, Daoling Peng, Fenglong Gu and Wencai Yi*



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Ground and excited state properties of ThB^- and ThB : a theoretical study

Isuru R. Ariyaratna

