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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

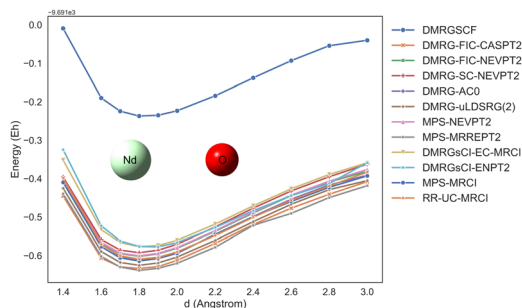
See Cercis Morera-Boado, Tina A. Harriott, Daniel Majaess, Chérif F. Matta *et al.*, pp. 12666–12674. Image reproduced by permission of Chérif F. Matta from *Phys. Chem. Chem. Phys.*, 2025, 27, 12666. Plot generated using data from Haoyu Fan *et al.*, 2019, *ApJ*, 878, 151

PERSPECTIVES

12622

Describing dynamic electron correlation beyond a large active space

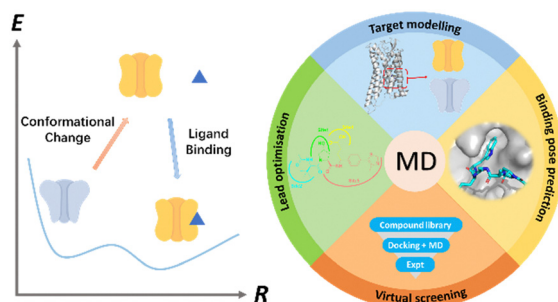
Yinxuan Song, Yifan Cheng* and Haibo Ma*



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Molecular dynamics-driven drug discovery

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



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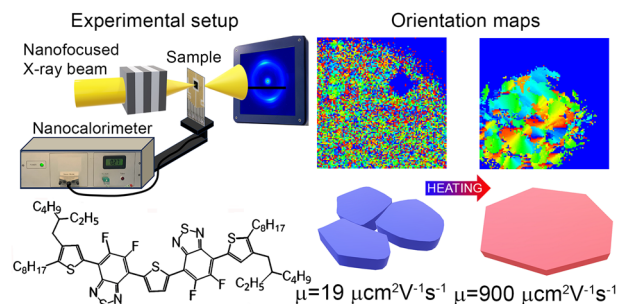


COMMUNICATION

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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. Akhkiamova, 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*

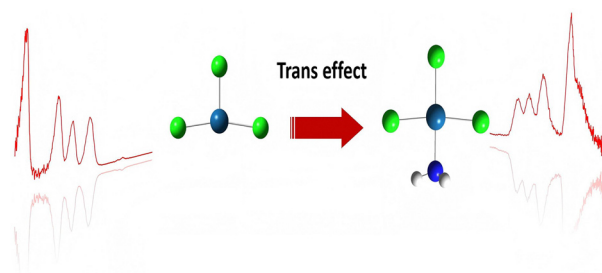


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Exploring the *trans* effect of the NH₃ ligand in platinum halide complexes Pt(NH₃)ClX₂[−] (X = Cl, Br, I) using cryogenic photoelectron spectroscopy and quantum chemical calculations

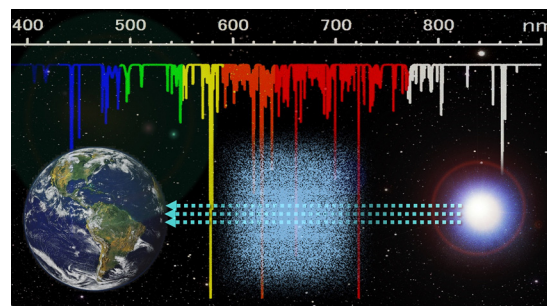
Qixu Zhao, Jian Zhang, Xueying Li, Peng Tang, Fan Yang, Junyang Ma, Zhubin Hu, Haitao Sun, Xue-Bin Wang,* Zhenrong Sun* and Yan Yang*



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

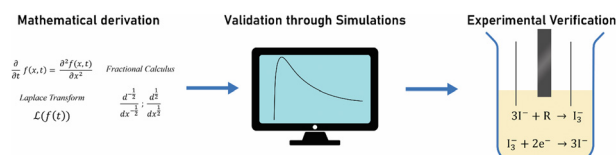
Halis Seuret, Ailish D. Sullivan, Cercis Morera-Boado,* Tina A. Harriott,* Daniel Majaess,* Lou Massa and Chérif F. Matta*



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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*



RESEARCH PAPERS

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VaporFit

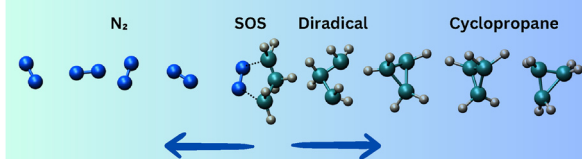
Software for Automated Atmospheric Correction in FTIR Spectroscopy

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

Przemysław Pastwa and Piotr Bruździak*

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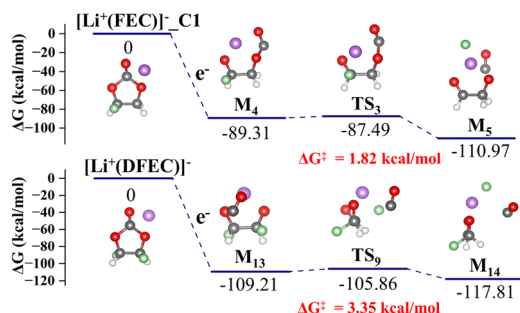
Post-second-order saddle dynamics



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

Renuka Pradhan and Upakarasamy Lourderaj*

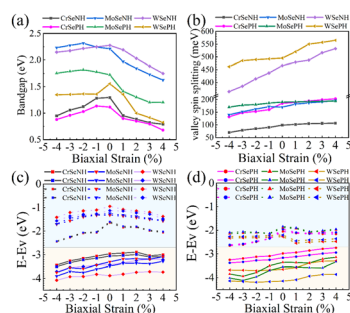
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Mechanistic insights into the thermodynamics and kinetics underlying the reductive decomposition of fluoroethylene and difluoroethylene carbonates for SEI formation in LIBs

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*

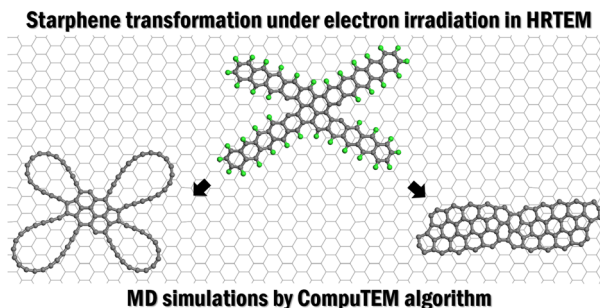


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Transformation of starphenes into amorphous graphene nanoribbons with attached carbon chains under electron irradiation

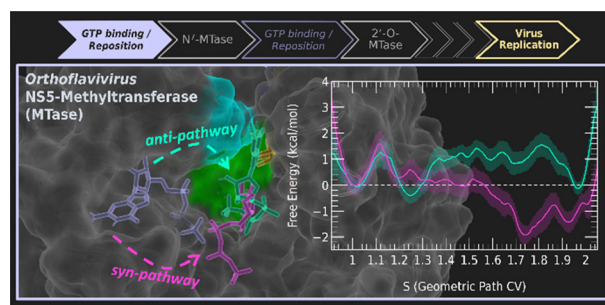
Alexander S. Sinitsa,* Yulia G. Polynskaya,
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Reposition pathways of GTP in *orthoflavivirus* NS5-methyltransferase revealed by enhanced molecular dynamics simulations

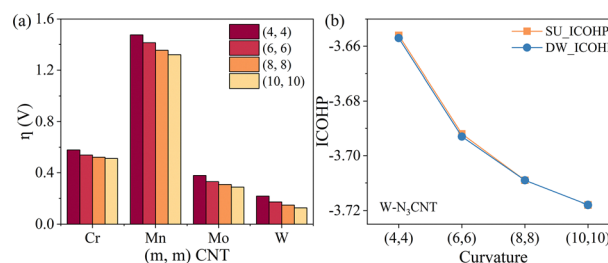
Lok Wan Ng, Yuen-Kit Cheng,
Wei Shen Aik* and Wei Han*



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

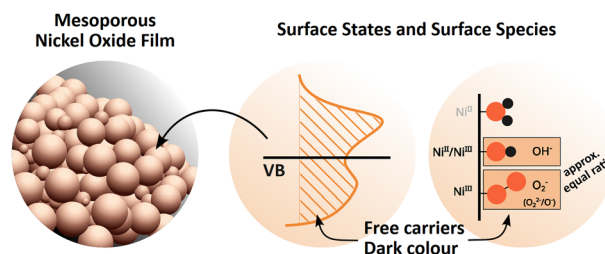
Xiaolin Jiang, Hongchang Xu, Lifu Zhang and
Zhenpeng Hu*



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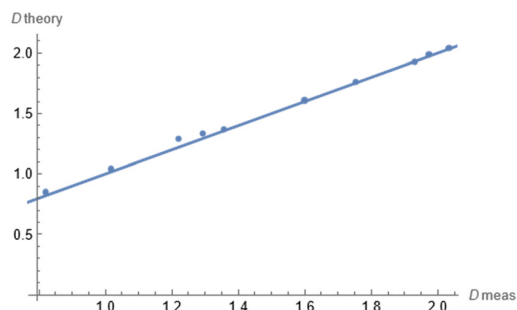
Insights into the surface of mesoporous nickel oxide and its interaction with oxygen and water

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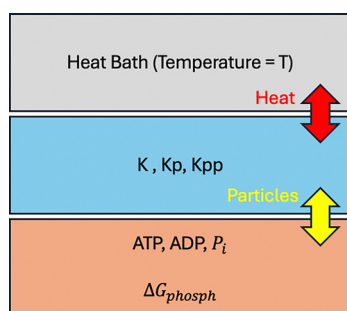
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The Poisson equation and polarization charge density in the concentration gradient of a diffusing electrolyte

Gerald S. Manning

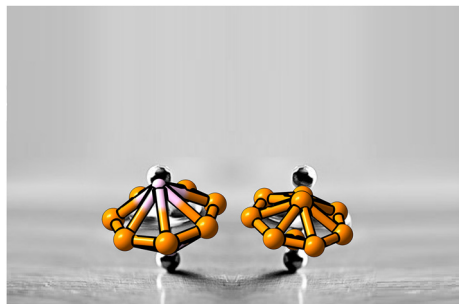
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Fluctuating signal and reversibility limit information and entropy in a MAPK signalling cascade

Harshita Saxena and Rati Sharma*

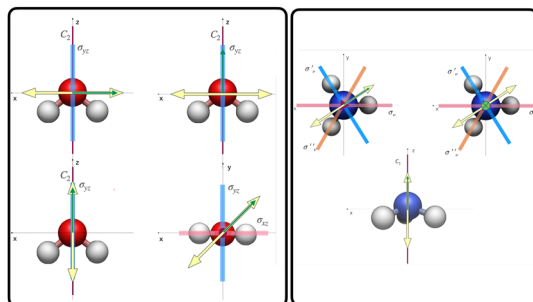
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Al₂B₇: an extension of the inverse sandwich B₉ cluster featuring Lewis acid sites and planar aromaticity

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

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

Marco Marchetta, Eleonora Luppi* and Emanuele Coccia*

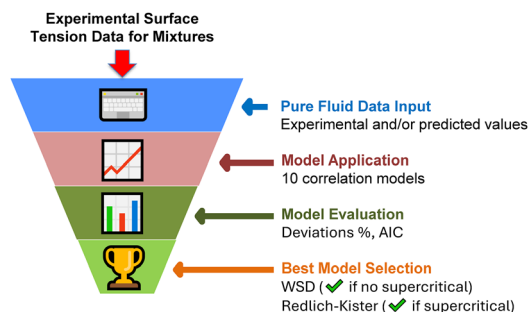


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Correlations of surface tension for mixtures of *n*-alkanes as a function of the composition: applicability and performance analysis of existing models

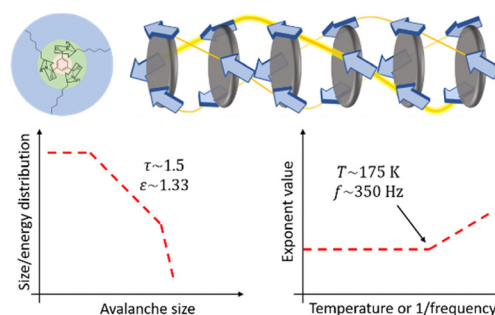
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Virginia Vadillo-Rodríguez and Isidro Cachadiña



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Barkhausen noise in the columnar hexagonal organic ferroelectric BTA

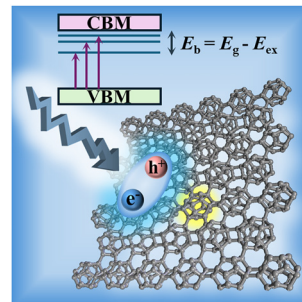
Andrey Alekseevich Butkevich, Fabian T. Thome,
Toni Seiler, Marcel Hecker and Martijn Kemerink*



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Pronounced excitonic effects in two-dimensional fullerene-based monolayer materials

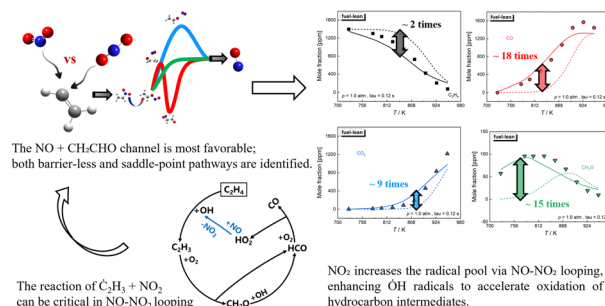
Ning Li, Tianqi Bao, Yang Zhao, Fan Zhang,
Junfeng Zhang, Xue Jiang, Nikolai Cherenda,
Weiwei Gao,* Jijun Zhao and Yan Su*



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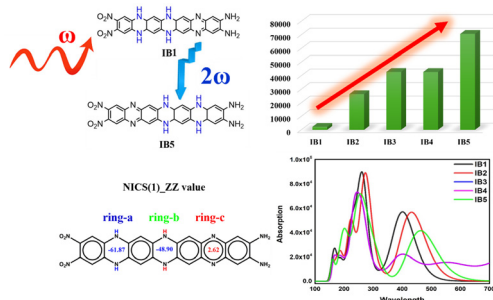
New insights into the kinetics of the reaction of vinyl radical with nitrogen dioxide

Qian Zhao,* Chunyu Wang, Yingjia Zhang,*
Huang Zuohua and Yuchun Zhang



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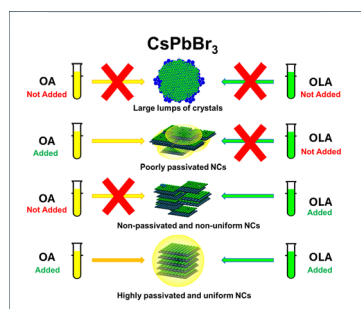
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Exploring the role of H-migration in the aromaticity, spectroscopic, photovoltaic and optical properties of planar heterocyclic compounds: a DFT study

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

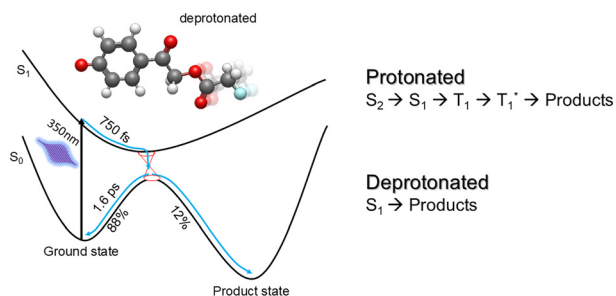
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Striking the balance between the capping ligands for CsPbBr₃ nanocrystal synthesis *via* an emulsion LARP approach

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

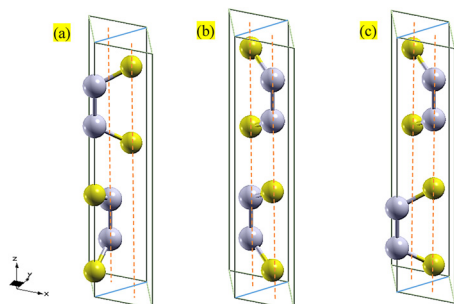
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pH-dependent ultrafast photodynamics of *p*-hydroxyphenacyl: deprotonation accelerates the photo-uncaging reaction

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

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

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

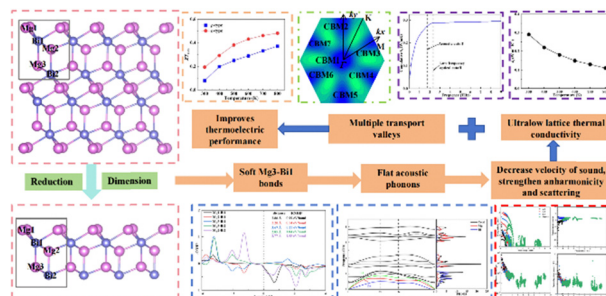


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Unraveling the lattice thermal conductivity and thermoelectric properties of monolayer Mg_3Bi_2

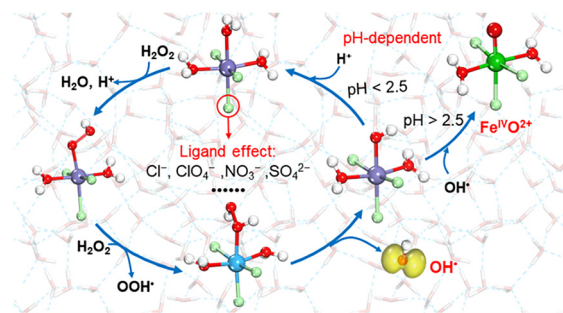
Yingying Chen, Zheng Ma, Na Zhao, Yajun Li, Xi Yao and Xilong Dou*



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

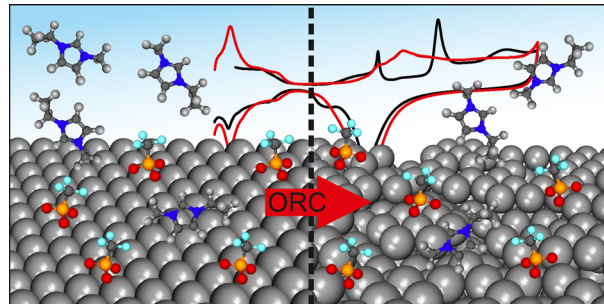
Ying Liu, Peijun Hu and Haifeng Wang*



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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

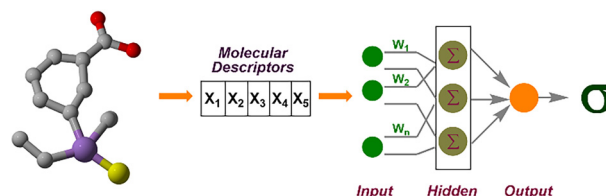
Felix Hilpert, Yunsheng Qiu, Leopold Lahn, Kevin Höllring, Nicola Taccardi, Peter Wasserscheid, Olga Kasian, Ana-Sunčana Smith, Karl J. J. Mayrhofer, Valentin Briega-Martos, Serhiy Cherevko, Olaf Brummel* and Jörg Libuda



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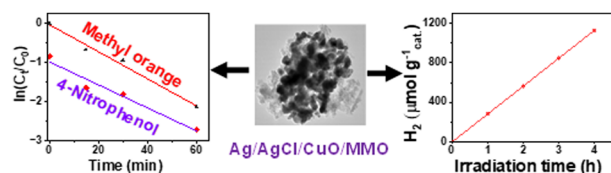
A machine learning-driven prediction of Hammett constants using quantum chemical and structural descriptors

Vaneet Saini* and Ranjeet Kumar



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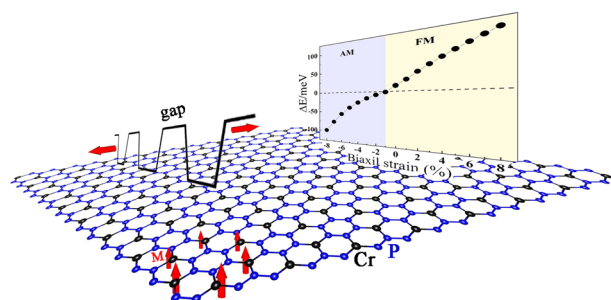
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Hierarchical microspheres of a mixed metal oxide heterojunction with CuO and Ag/AgCl for enhanced photocatalytic oxidation of organic pollutants and hydrogen production

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

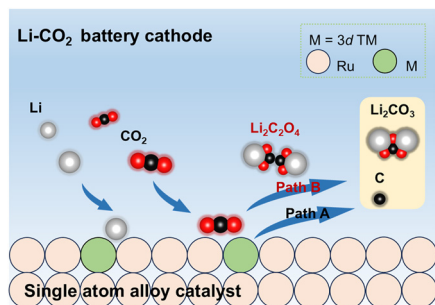
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Magnetic switching and quantization of bandgap in 2D graphene-like CrP₃

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

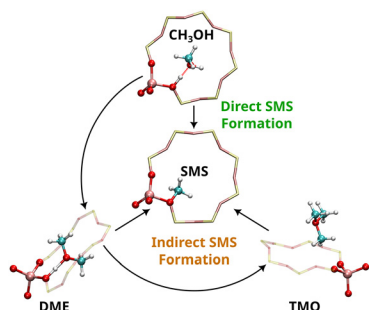
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Promising Ru-based cathode catalysts for Li–CO₂ batteries via single-atom alloying

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*

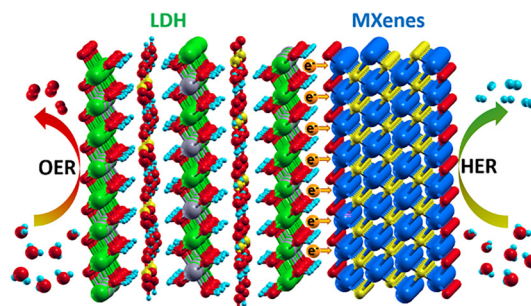


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MXenes enhance electrocatalytic water electrolysis of NiFe layered double hydroxides through bifunctional heterostructuring

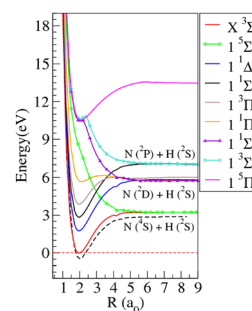
Nannan Li, Xiaotong Han, Ho Seok Park and Jin Yong Lee*



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

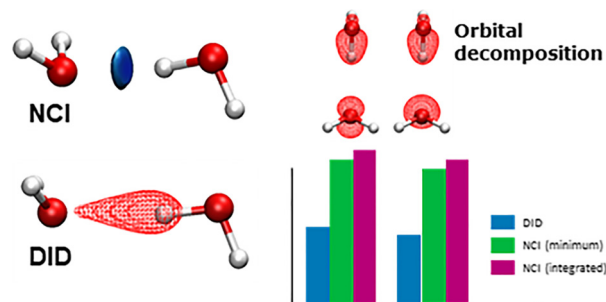
Raju Ghosh, Binayak Samaddar Choudhury, János Zsolt Mezei, Ioan F. Schneider, Nicolina Pop and Kalyan Chakrabarti*



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NCI orbital decomposition and critical comparison to local correlation schemes

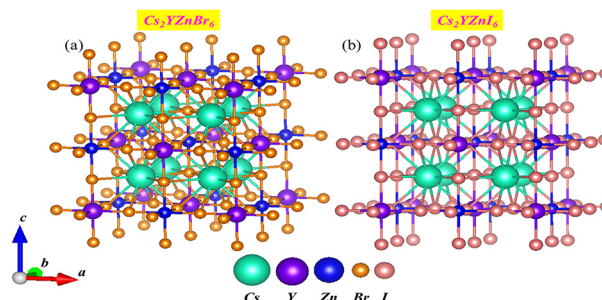
Xaiza Aniban, Maxime Ferrer, M. Merced Montero-Campillo, Ricardo A. Mata,* Julia Contreras-García* and Martí Gimferrer*



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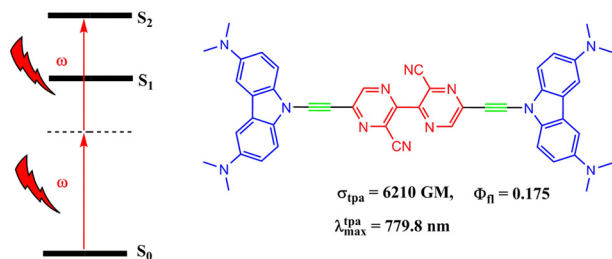
First principles insight into Cs₂YZnX₆ (X = Br, I) double perovskite materials for optoelectronic and thermoelectric device applications

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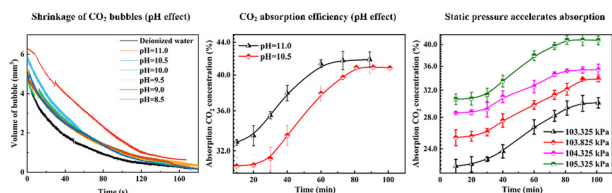
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Theoretical study of the two-photon absorption and fluorescence emission properties of bipyrzine (or hexaazatriphenylene) core based donor- π -acceptor- π -donor framework chromophores

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

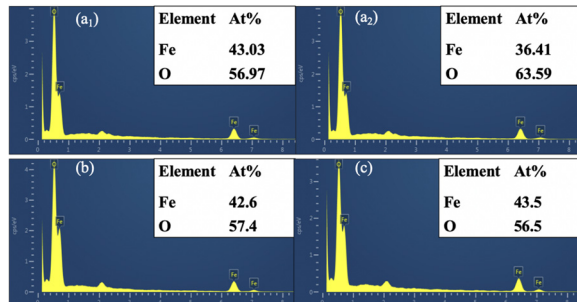
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Study on the mass transfer behavior of single CO₂ bubbles in sodium silicate solution

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

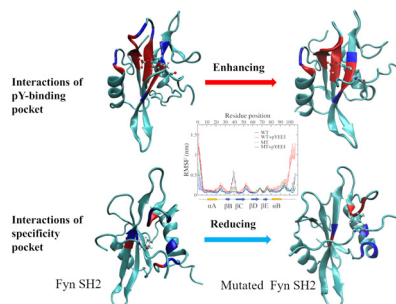
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Preparation of non-spherical nano-Fe₃O₄ and its effect on thermal decomposition of AP and combustion performance of composite fuels

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*

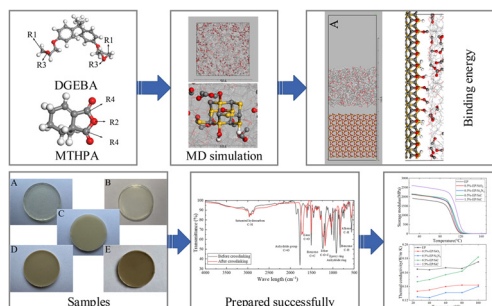


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A study on the thermodynamic performance of nano-silicide filled epoxy resin composite materials

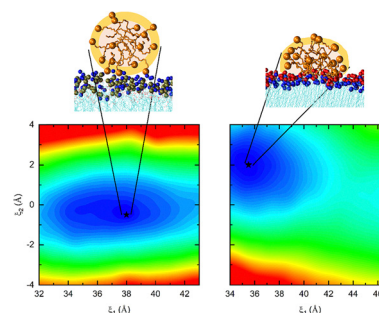
Hang Zhang, Zhijin Zhang,* Chao Liu, Xingliang Jiang, Jianlin Hu and Qin Hu



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

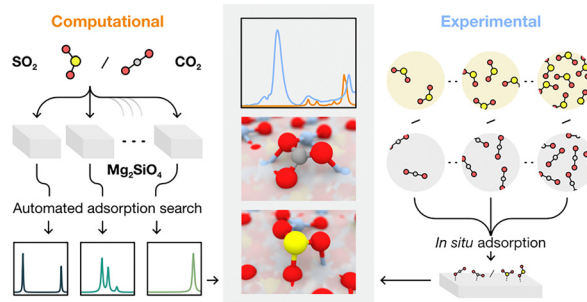
Yeonho Song and Hyonseok Hwang*



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

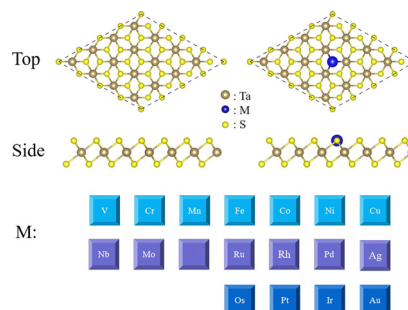
Eric Mates-Torres,* Guillermo Escolano Casado, Lorenzo Mino,* Nadia Balucani, Piero Ugliengo and Albert Rimola*



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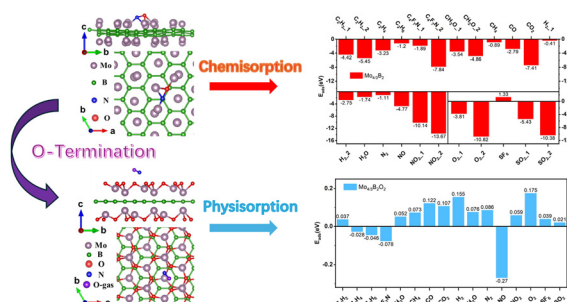
Computational screening of transition-metal atom embedding in 1T-TaS₂ monolayer defects as efficient oxygen-reduction/evolution-reaction bifunctional catalysts

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



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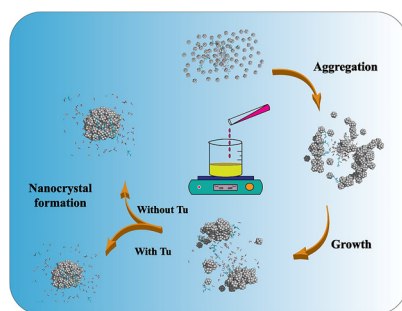
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Achieving tunable adsorption selectivity and sensitivity of boridenes for gas detection by surface O-termination engineering

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

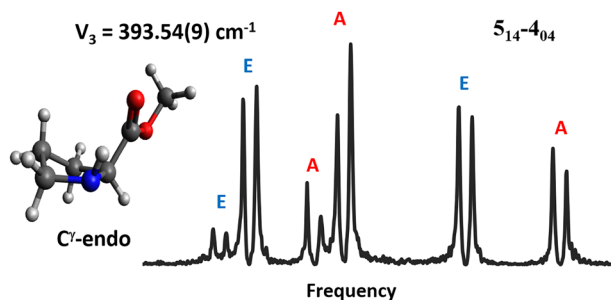
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Mechanistic insights on sulfur functionalization of Ag nanoflowers

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

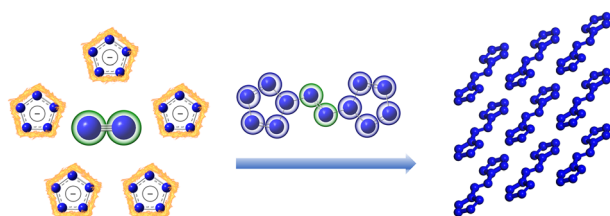
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The challenging conformer assignment of proline methyl ester from rotational spectroscopy

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 $\pi-\pi$ 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

