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REVIEW

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Contemporary DFT: learning from traditional and recent trends for the development and assessment of accurate exchange–correlation functionals

E. Brémond, A. J. Pérez-Jiménez, C. Adamo and J. C. Sancho-García*

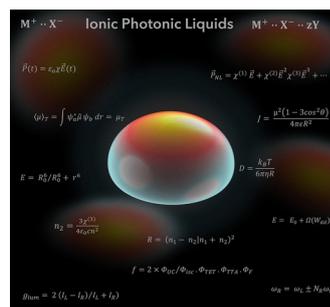


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Neat ionic liquids and deep eutectic solvents in photonics: *status quo* and future directions

Mila Miroschnichenko and Pankaj Bharmoría*



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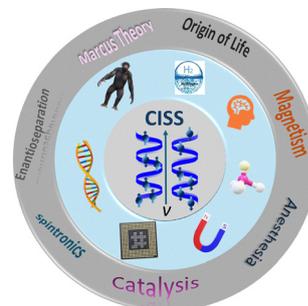
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PERSPECTIVES

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Chirality-induced spin selectivity: an interdisciplinary perspective from chemical physics to biology

Anil Kumar* and Anu Gupta*



COMMUNICATION

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Eutectic solvent as electrolytes for rechargeable proton batteries

Masahiro Shimizu,* Tomonori Ichikawa, Shino Goto and Yasunori Toda

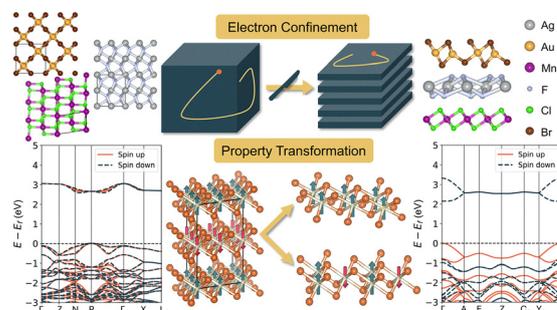


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A first-principles theoretical study on two-dimensional MX and MX₂ metal halides: bandgap engineering, magnetism, and catalytic descriptors

Yu-Hsiu Lin, Daniel Maldonado-Lopez and Jose L. Mendoza-Cortes*



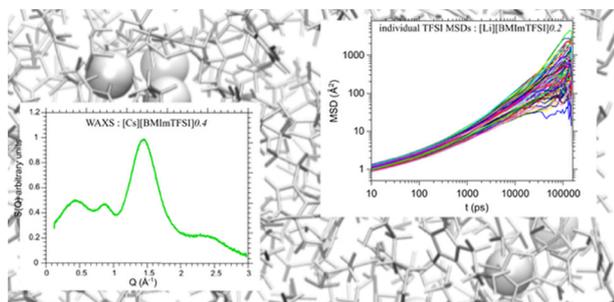
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Ionic liquid conductivity models by symbolic regression

Isak Bengtsson* and Patrik Johansson



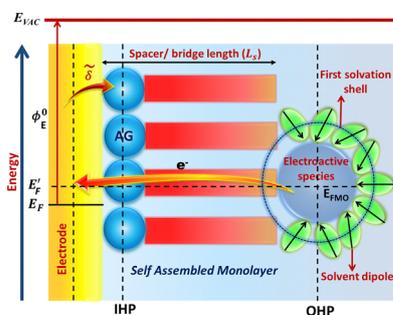
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Structural and dynamical heterogeneities at the nanoscale in alkali/earth alkaline ionic liquid electrolytes: experiment and molecular simulation

Patrick Judeinstein,* Hoang Phuong Khanh Ngo, Fabrice Cousin, Cristina Iojoiu, Emilie Planes and Benoît Coasne*

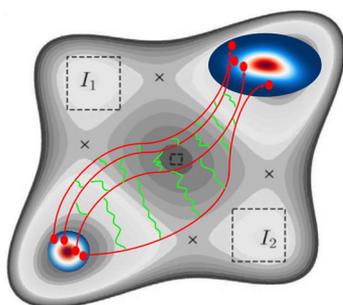
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Theory for heterogeneous electron transfer in self-assembled monolayers on metal electrodes

Neha Yadav and Rama Kant*

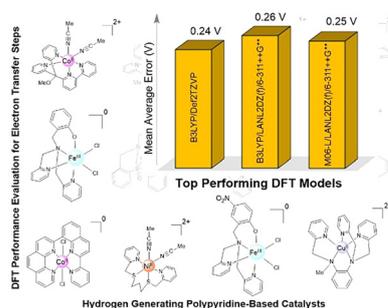
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Quantum dynamical concertedness: an entangled trajectory molecular dynamics study

Aanchal Grover and Srihari Keshavamurthy*

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How reliable is DFT for predicting the redox potentials in polypyridine-based hydrogen evolution catalysts?

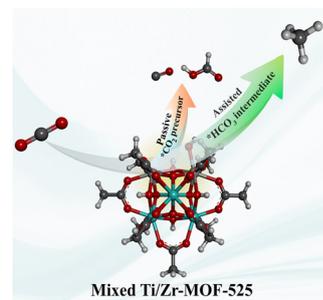
Sheetal Ranaut and Shivnath Mazumder*



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CO₂ photoreduction on mixed Ti/Zr-MOF-525: bicarbonate as the active intermediate and the role of Ti substitution

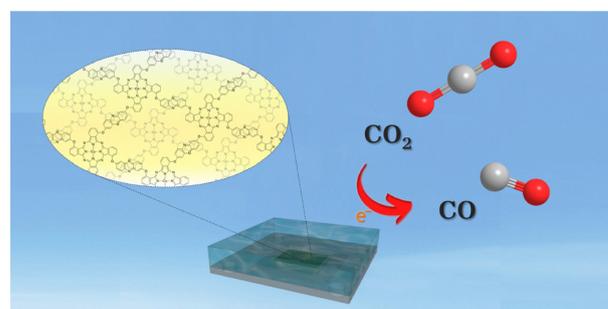
Thanyaporn Puengpoka, Jirapat Santatiwongchai, Warot Chotpatiwetchkul,* Sareeya Bureekaew, Muhammad Saleh, Anchalee Junkaew and Sarawoot Impeng*



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A polymeric α -tetrasubstituted Co^{II}-phthalocyanine catalyst for stable and selective electrochemical carbon dioxide reduction

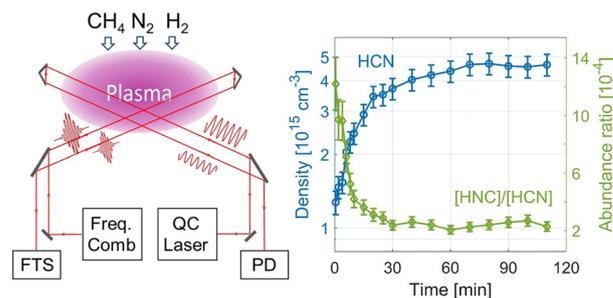
Kornkamol Mangmoon, Permsak Chairat, Yijiao Jiang, Poobodin Mano, Supawadee Namuangruk and Patchanita Thamyongkit*



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Formation of HNC and HCN isomers in molecular plasmas revealed by frequency comb and quantum cascade laser spectroscopy

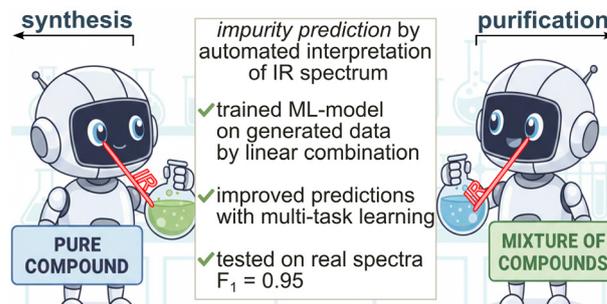
Ibrahim Sadiq,* Simona Di Bernardo, Uwe Macherius and Jean-Pierre H. van Helden



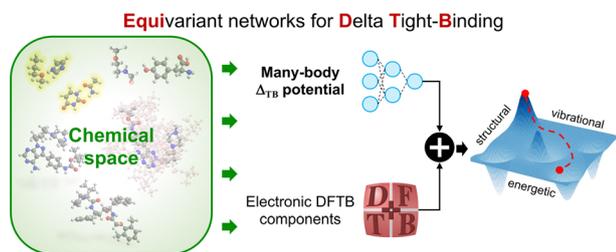
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Infrared spectroscopy-assisted prediction of impurities in chemicals using machine learning: towards smart self-driving laboratories

Anastasiia M. Kutskaia and Konstantin S. Rodygin*



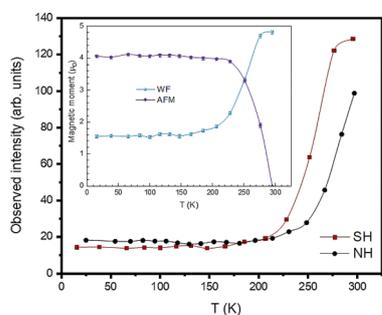
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Advancing density functional tight-binding method for large organic molecules through equivariant neural networks

Leonardo Medrano Sandonas,* Mirela Puleva, Zekiye Erarslan, Ricardo Parra Payano, Martin Stöhr, Gianaurelio Cuniberti and Alexandre Tkatchenko*

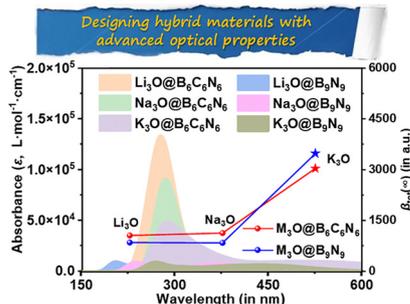
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Magnetism of nanostructured hematite: from cultural heritage to fundamental properties

Sawssen Slimani,* Alberto Martinelli, Alexander Omelyanchik, Maryam Abdolrahimi, Elena Castagnotto, Pierfrancesco Maltoni, Sara Laureti, Gianni Barucca, Nader Yaacoub, Federico Locardi, Arooj Ramzan, Laura Gaggero, Maurizio Ferretti and Davide Peddis

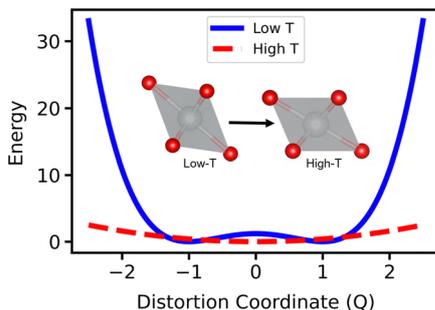
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Designing hybrid materials with advanced optical properties using superalkali M₃O (M = Li, Na, and K) and isoelectronic species of cyclo[18]carbon (B₆C₆N₆ and B₉N₉)

Xiaohui Chen, Xiufen Yan, Tian Lu and Zeyu Liu*

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First-principles investigation of the insulator–metal transition in layered NaNiO₂: coupled electronic and lattice effects

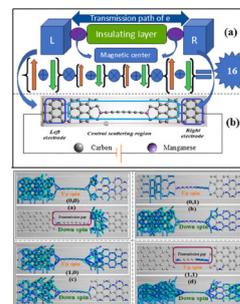
Xiaohong Chu, Zhenyi Jiang,* Ping Guo,* Jiming Zheng and Xiaodong Zhang



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First-principles study of spin-selective transport properties and quantum logic gate operation in transition-metal-capped nanowires

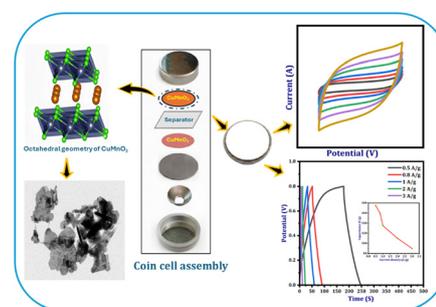
Dipankar Adak, Debnarayan Jana,*
Mausumi Chattopadhyaya and Sabyasachi Sen*



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Electrochemical study of crednerite CuMnO_2 for symmetric supercapacitor applications

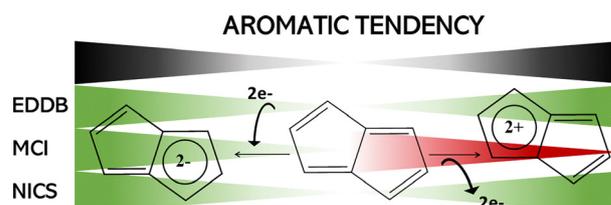
Karan S. Modi, Pruthvi B. Patel, Dharti Patel, Jay Patel,
Vanaraj Solanki* and Mitesh H. Patel*



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Expanding aromaticity tests to include lowest-lying triplet excited states and charged and heterocyclic rings

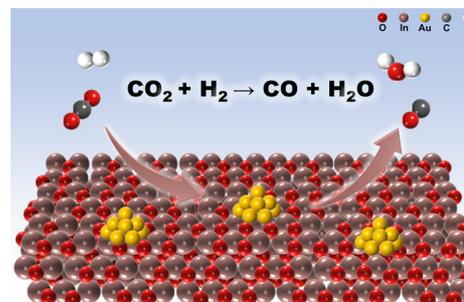
Maria Cabrero-Martí and Miquel Solà*



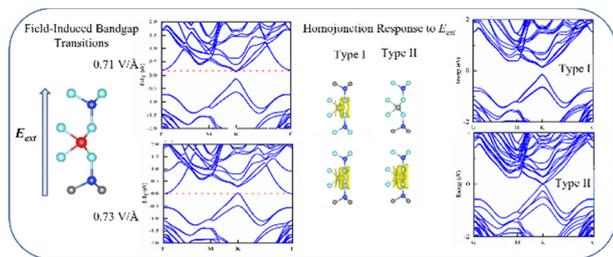
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A highly active $\text{Au}/\text{In}_2\text{O}_3$ catalyst for the reverse water gas shift reaction

Yuxue Zhao, Linlin Wu, Liangkai Xu, Rui Zou and
Chang-jun Liu*



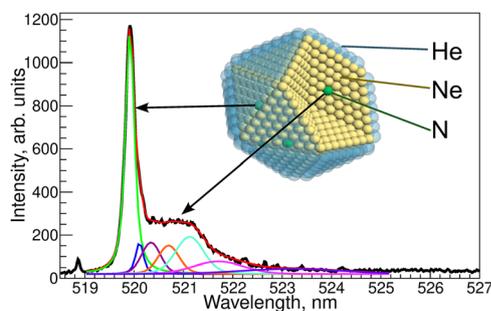
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Effects of an external electric field on the electronic properties of $MSi_2P_xAs_y$ monolayers and homojunctions: a first-principles study

Long Lai, Jianwei Wang* and Xiaobin Niu*

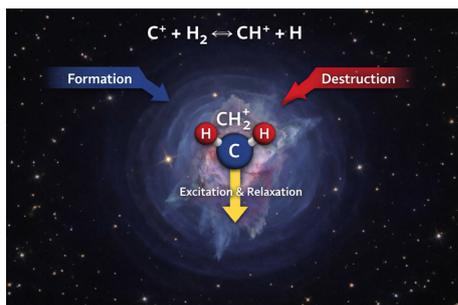
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Influence of solid helium on the luminescence of nitrogen–neon nanoclusters

Oleksandr Korostyshevskiy,* Cameron K. Wetzel, David M. Lee and Vladimir V. Khmelenko

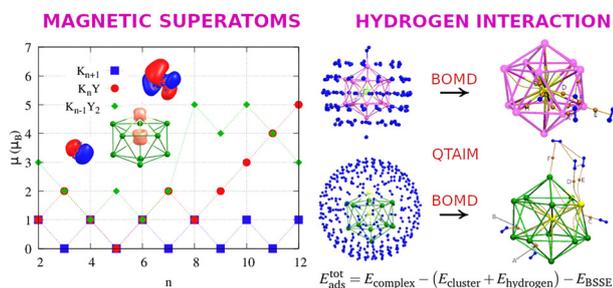
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Rate constants for a reactive system of astrophysical interest: a statistical study of CH_2^+

Tomás González-Lezana,* Maarten Konings, Jérôme Loreau, François Lique, Milan Sil and Alexandre Faure

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Yttrium-doped lithium and potassium clusters: magnetic superatoms and their interaction with hydrogen

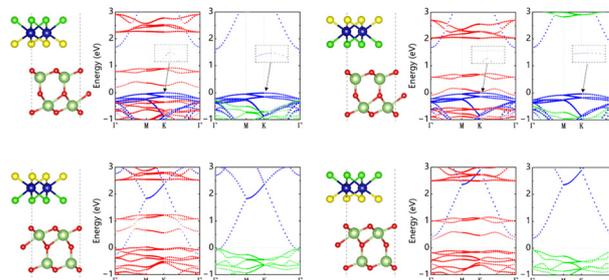
Henry Nicole González-Ramírez,* Zeferino Gómez-Sandoval,* Gururaj Kudur Jayaprakash, Juan Pablo Mojica-Sánchez, Roberto Flores-Moreno and Kayim Pineda-Urbina



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Electronic and magnetic properties modulated by nonvolatile switching in the multiferroic $\text{Cr}_2\text{Cl}_3\text{S}_3/\text{Ga}_2\text{O}_3$ van der Waals heterostructure

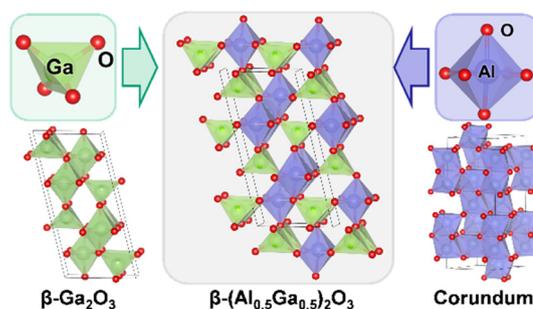
Jing-Jing He, Jun-Yi Gu, Qin-Yue Cao, Ling-Xiao Liu, Min Hua, Jia-Ren Yuan,* Yan-Dong Guo* and Xiao-Hong Yan*



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The electronic structures of β -phase $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$ studied using DFT calculations

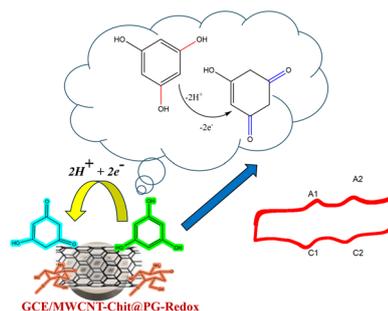
Ziqian Sheng, Wenjing Xu, Xiaoqing Zhou, Cien Liu, Alexander Polyakov, Zhilai Fang, Ning Jia,* Xiangyu Xu* and Kelvin H. L. Zhang*



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Designing *in situ* nanostructured MWCNT-phloroglucinol modified webs for electrochemical-based dual screening of stress biomarkers

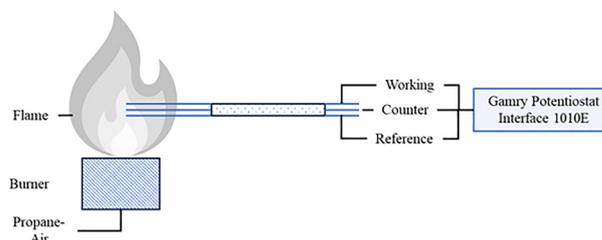
Mansi Gandhi and Anitha Varghese*



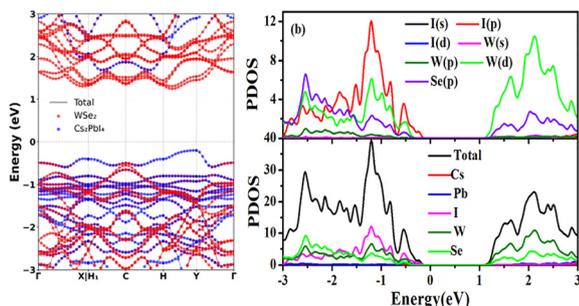
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Electrochemistry in flame plasmas: passive films and impedance analysis

Bill Logan Riehl* and Craig E. Banks



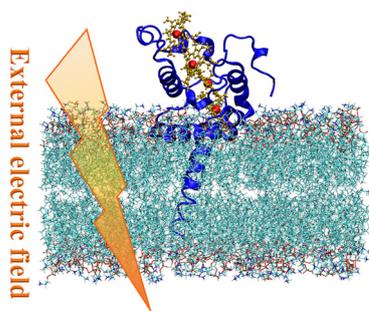
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Insight into the photoelectric characteristics and photocatalytic water splitting performances of van der Waals heterostructures $\text{Cs}_2\text{PbI}_4/\text{MX}_2$ ($\text{M} = \text{Mo}, \text{W}$; $\text{X} = \text{Se}, \text{S}$)

Wei-Bing Zhang, Ai-Jie Mao,* Hua-Yun Geng and Xiang-Rong Chen*

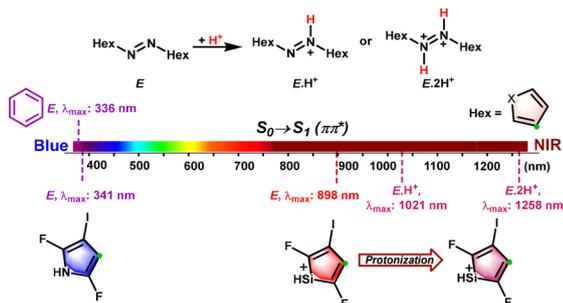
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Electrostatic and proton–electron interaction in membrane-bound charge transfer proteins under external electric fields: a computational study

Zeinab Rahimi, Amir Lohrasebi* and Thorsten Koslowski

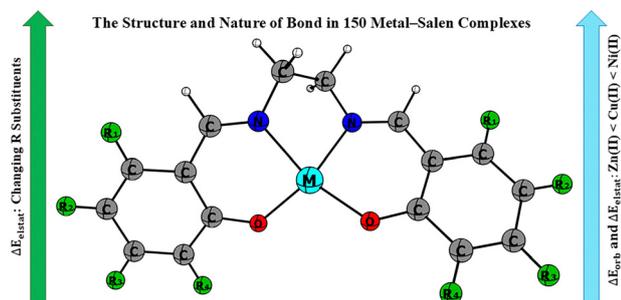
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Probing the longest λ_{max} of azo compounds in near infrared absorption via integrating protonation, antiaromaticity and substituents: a combined DFT and machine learning study

Shuwen Chen, Yuan Gao, Wenhao Wang and Jun Zhu*

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Theoretical studies on the strength and nature of the bond in Ni(II), Cu(II) and Zn(II) complexes of a large series of symmetric salen ligands

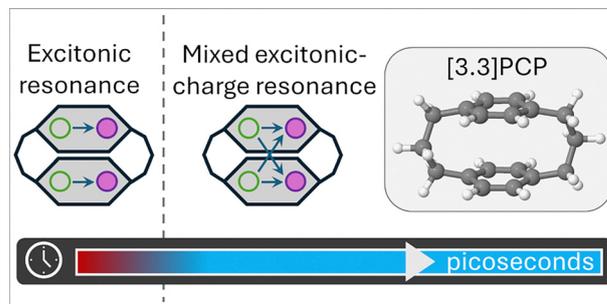
Seyedeh Aghigh Hamrahian, Samaneh Sanei Movafagh and Sadegh Salehzadeh*



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Ultrafast dynamics and excited-state trapping in [3.3]paracyclophane

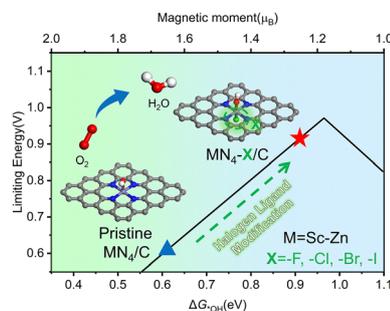
Muhammad Tahir Hafeez, Rafael S. Mattos, Lea M. Ibele* and Mario Barbatti*



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Impact of halogen axial coordination on the electronic and magnetic properties of MN_4 single-atom catalysts for oxygen reduction

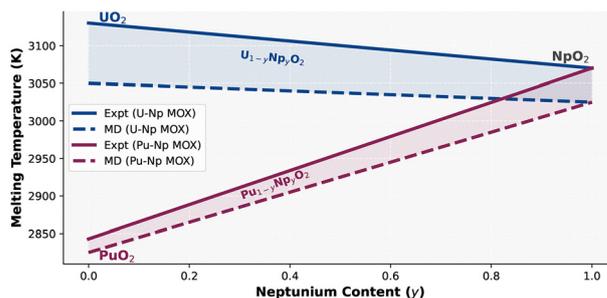
Bo-Yang Luo, Chen Li, Yu-Mei Yang, Wei Du and Ya-Min Wang*



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High temperature thermal and melting properties of uranium–neptunium and plutonium–neptunium mixed oxides: a MD simulation study

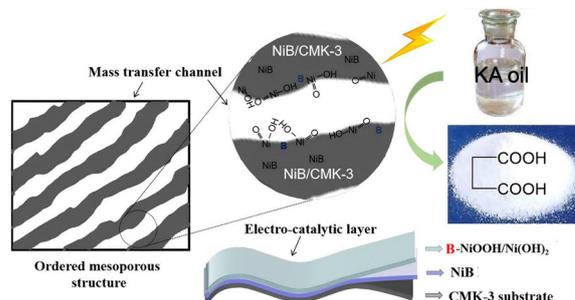
A. Chakraborty, N. Choudhury* and P. S. Ghosh*



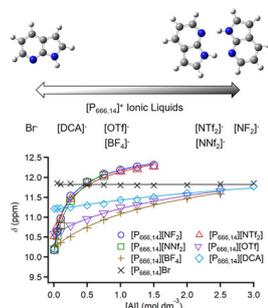
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Amorphous NiB as an electrocatalyst: from KA oil to succinic acid

Yulin Zhou,* Lei Zhu, Xiaohong Tao, Wenbin Jiang, Jun Chai* and Hangjia Shen*



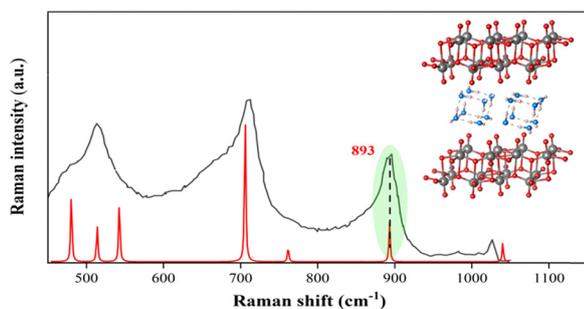
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Dimer formation of 7-azaindole in phosphonium-based ionic liquids: anion-dependent behavior

Faruk Hossain, Kotaro Takahashi, Maharoo Koyakkat and Hideaki Shirota*

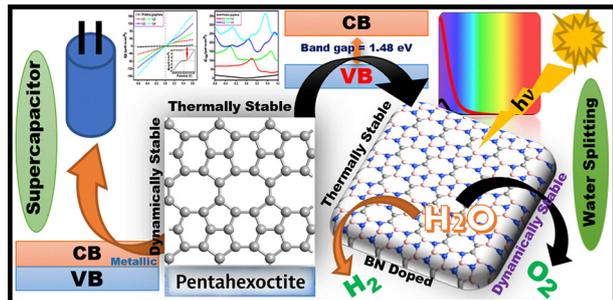
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A comparative theoretical study on the vibrational spectra of $V_2O_5 \cdot nH_2O$

Shuang Yu, Xiaodong Zhang, Qiang Zhan, Hao Yu and Bo Zhou*

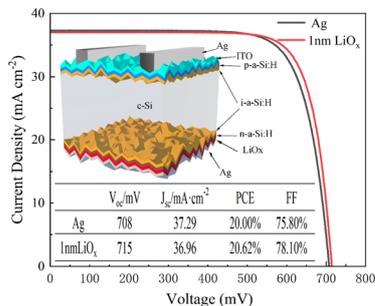
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Theoretical insights into the structural, electronic, photocatalytic and supercapacitor applications of pentahexoctite

Nirmal Barman and Utpal Sarkar*

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Ultralow-work-function lithium oxide (LiO_x) as electron-selective contact for silicon heterojunction solar cell

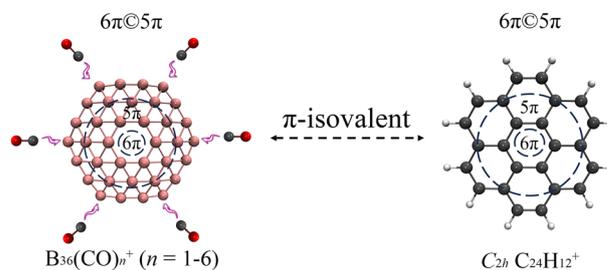
Yusen Lin, Zhi Xu, Zhenjia Wang, Xuanfei Kuang, Yao Xiao, Zijing Wang, Xipeng Zhang and Zongcun Liang*



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Observation of quasi-planar boron carbonyl complexes $B_{36}(CO)_n^+$ ($n = 1-6$) analogous to coronene monocation $C_{24}H_{12}^+$

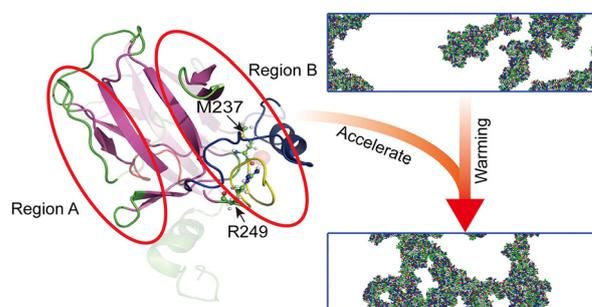
Hong Niu, Qiang Chen,* Qin-Wei Zhang, Xi Chen, Teng Li, Xiao-Ni Zhao and Si-Dian Li*



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The molecular mechanism of temperature-dependent p53C phase separation accelerated by oncogenic mutations: insights from all-atom and coarse-grained molecular dynamics simulations

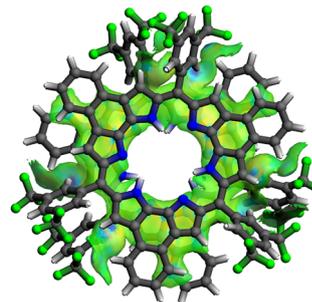
Zhifa Duan, Yi Song, Huanhuan Ruan, Tianjing Guo and Jiangtao Lei*



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Insights into the intermolecular interactions between stacked antiaromatic 24- π hexaphyrin macrocycles: variation of the magnetic response properties

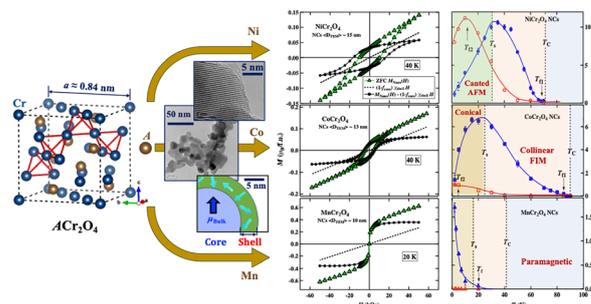
Alvaro Muñoz-Castro



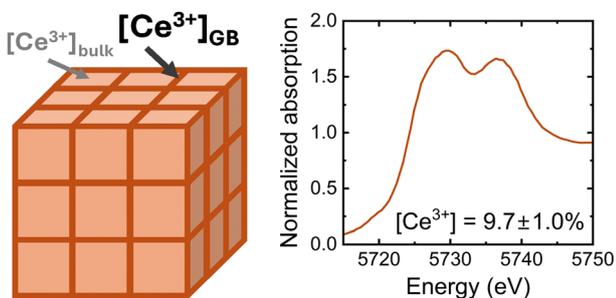
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Structural, optical, and magnetic properties with finite-size and interface effects of noncollinear ferrimagnetic ACr_2O_4 ($A = Ni, Co, \text{ and } Mn$) single-domain nanocrystals

Mohamed A. Kassem,* Ahmed M. Nashaat and Abdulaziz Abu El-Fadl



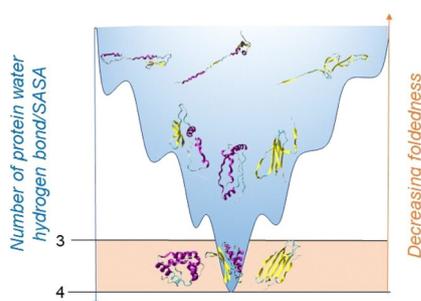
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Direct *in situ* detection of grain boundary reduction in nanocrystalline ceria

Claire M. Donahue, Qing Ma and Sossina M. Haile*

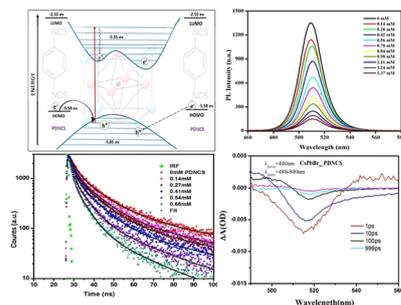
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Solvent accessible surface area normalized protein–water hydrogen bonds define protein folded state stability and amyloid formation

Prasun Pal, Rahul Debnath, Biman Jana* and Sandipan Chakraborty*

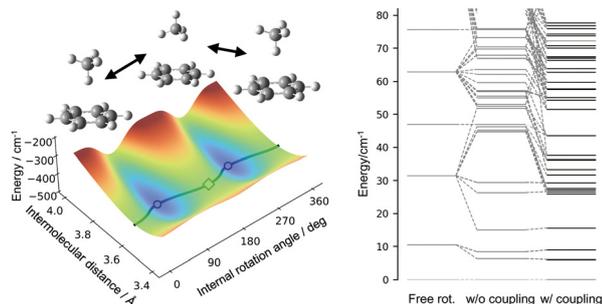
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Hole transfer dynamics between CsPbBr₃ PNCs and *p*-phenylene diisothiocyanate

Sourav Mandal, Subhadip Giri, Suraj Barman, Sourav Nandi, Shashanka Shekhar Samanta, Sayan Prodhan, Ayon Jyoti Karmakar, Prasanta Kumar Datta and Ajay Misra*

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Six-dimensional intermolecular potential energy surface and vibrational states of the benzene–methane vdW complex

Toru Sasaki, Masaaki Nakamura and Yasuhiro Ohshima*

