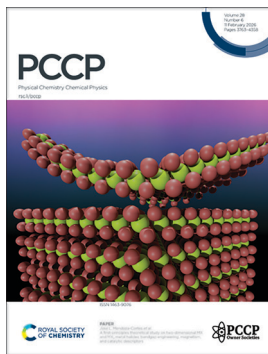


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### Cover

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

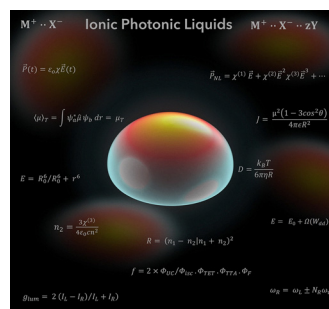


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### Neat ionic liquids and deep eutectic solvents in photonics: *status quo* and future directions

Mila Miroschnichenko and Pankaj Bharmoria\*



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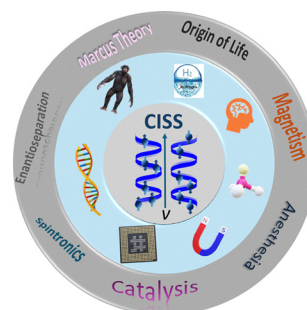
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## Chirality-induced spin selectivity: an interdisciplinary perspective from chemical physics to biology

Anil Kumar\* and Anu Gupta\*

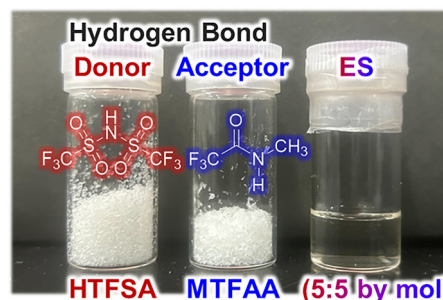


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## Eutectic solvent as electrolytes for rechargeable proton batteries

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

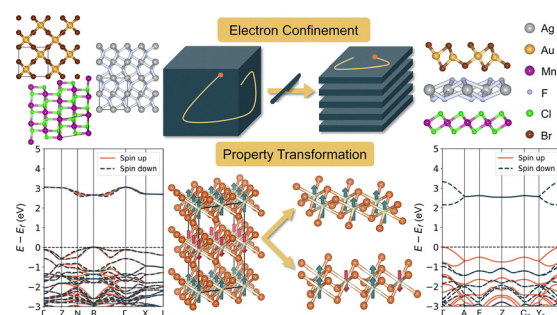


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A first-principles theoretical study on two-dimensional MX and MX<sub>2</sub> metal halides: bandgap engineering, magnetism, and catalytic descriptors

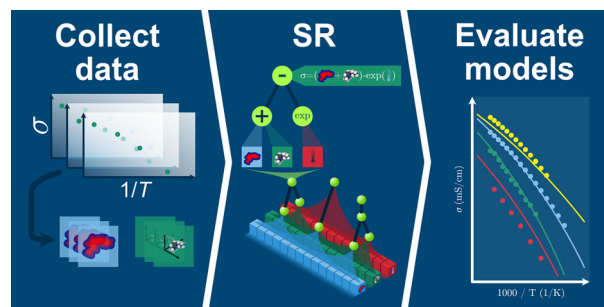
Yu-Hsiu Lin, Daniel Maldonado-Lopez and Jose L. Mendoza-Cortes\*



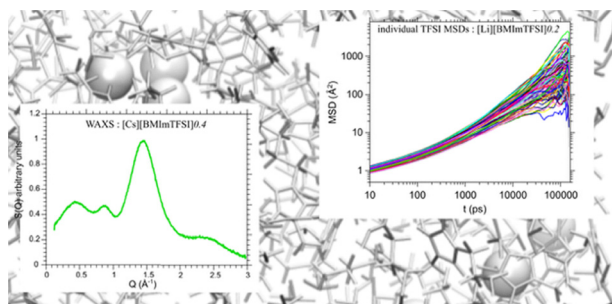
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## Ionic liquid conductivity models by symbolic regression

Isak Bengtsson\* and Patrik Johansson



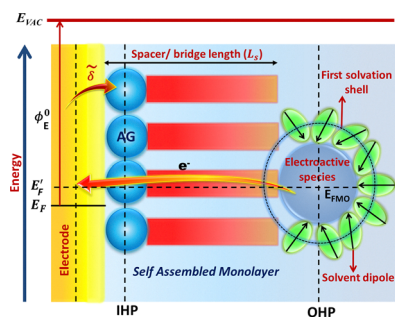
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### Structural and dynamical heterogeneities at the nanoscale in alkali/earth alkaline ionic liquid electrolytes: experiment and molecular simulation

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

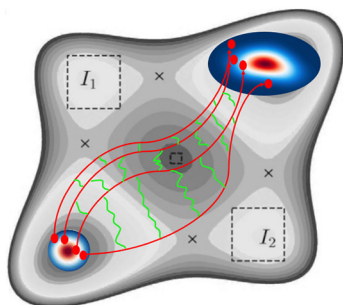
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### Theory for heterogeneous electron transfer in self-assembled monolayers on metal electrodes

Neha Yadav and Rama Kant\*

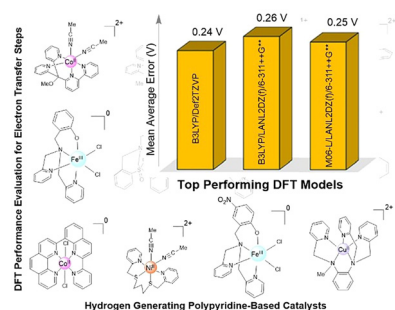
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### Quantum dynamical concertedness: an entangled trajectory molecular dynamics study

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\*

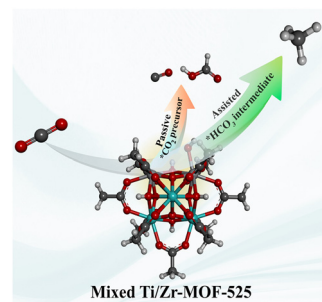


## RESEARCH PAPERS

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**CO<sub>2</sub> photoreduction on mixed Ti/Zr-MOF-525: bicarbonate as the active intermediate and the role of Ti substitution**

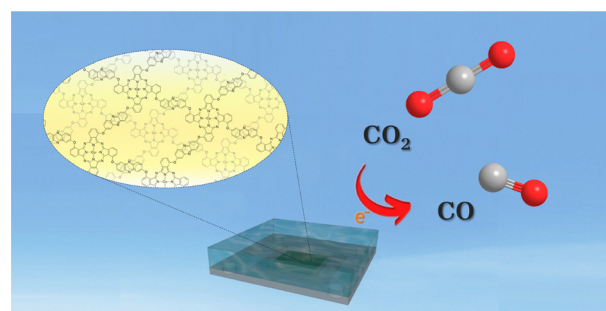
Thanyaporn Puengpoka, Jirapat Santatiwongchai, Warot Chotpatiwetchkul,\* Sareeya Bureekaew, Muhammad Saleh, Anchalee Junkaew and Sarawoot Impeng\*



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**A polymeric  $\alpha$ -tetrasubstituted Co<sup>II</sup>-phthalocyanine catalyst for stable and selective electrochemical carbon dioxide reduction**

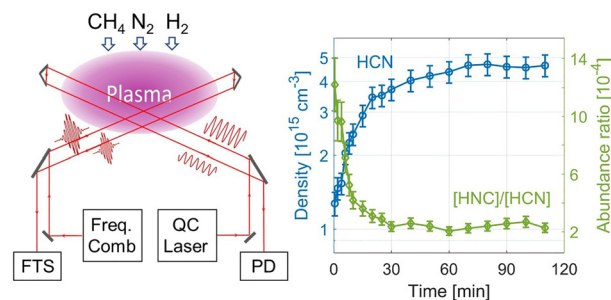
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**Formation of HNC and HCN isomers in molecular plasmas revealed by frequency comb and quantum cascade laser spectroscopy**

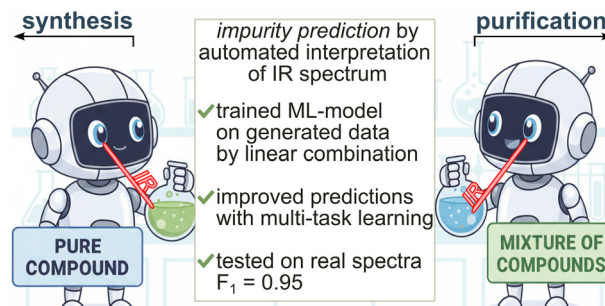
Ibrahim Sadiq,\* Simona Di Bernardo, Uwe Macherius and Jean-Pierre H. van Helden



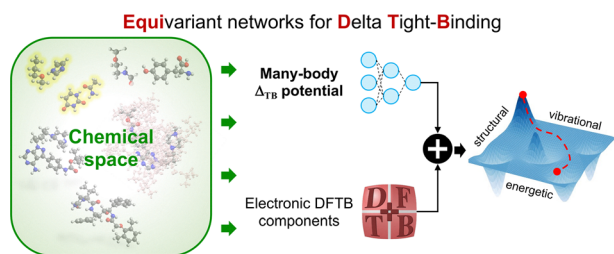
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**Infrared spectroscopy-assisted prediction of impurities in chemicals using machine learning: towards smart self-driving laboratories**

Anastasiia M. Kutskaia and Konstantin S. Rodygin\*



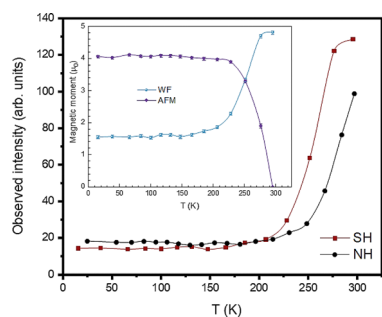
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### Advancing density functional tight-binding method for large organic molecules through equivariant neural networks

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

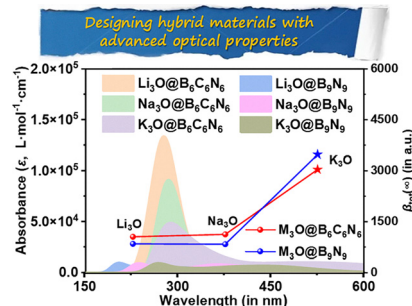
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### Magnetism of nanostructured hematite: from cultural heritage to fundamental properties

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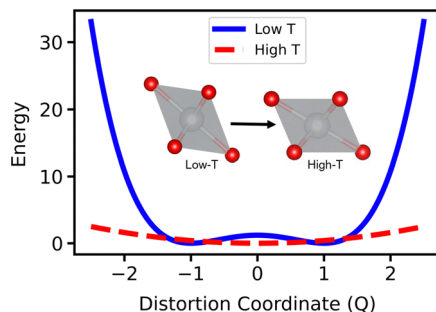
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### Designing hybrid materials with advanced optical properties using superalkali $M_3O$ ( $M = \text{Li}, \text{Na}, \text{and K}$ ) and isoelectronic species of cyclo[18]carbon ( $B_6C_6N_6$ and $B_9N_9$ )

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

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### First-principles investigation of the insulator–metal transition in layered $\text{NaNiO}_2$ : coupled electronic and lattice effects

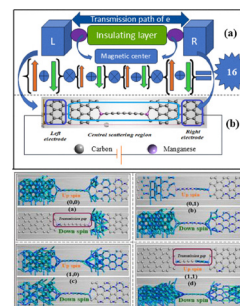
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### First-principles study of spin-selective transport properties and quantum logic gate operation in transition-metal-capped nanowires

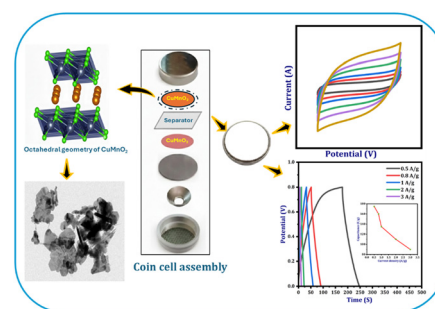
Dipankar Adak, Debnarayan Jana,\*  
Mausumi Chattopadhyaya and Sabyasachi Sen\*



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### Electrochemical study of crednerite $\text{CuMnO}_2$ for symmetric supercapacitor applications

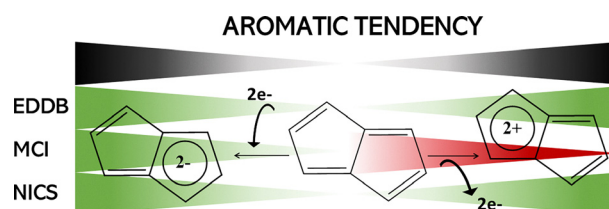
Karan S. Modi, Pruthvi B. Patel, Dharti Patel, Jay Patel,  
Vanaraj Solanki\* and Mitesh H. Patel\*



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

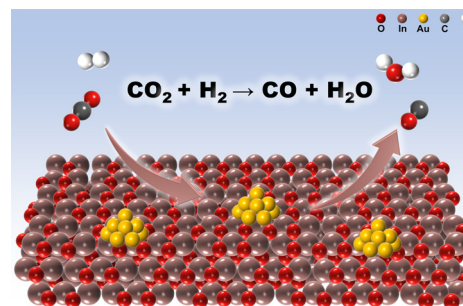
Maria Cabrero-Martí and Miquel Solà\*



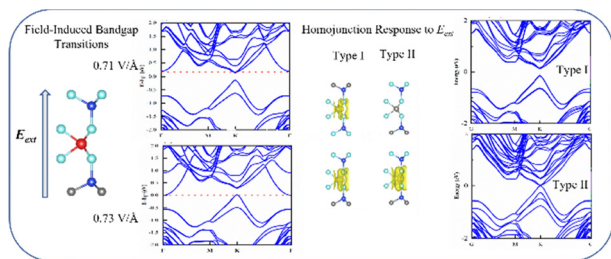
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### A highly active $\text{Au}/\text{In}_2\text{O}_3$ catalyst for the reverse water gas shift reaction

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



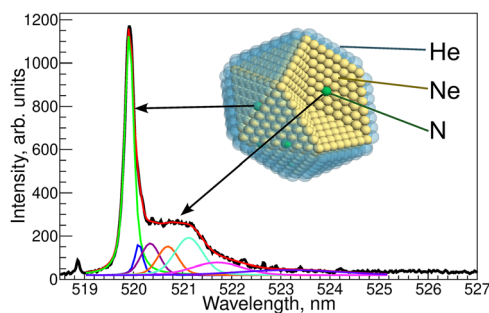
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### Effects of an external electric field on the electronic properties of $MSi_2P_xAs_y$ monolayers and homojunctions: a first-principles study

Long Lai, Jianwei Wang\* and Xiaobin Niu\*

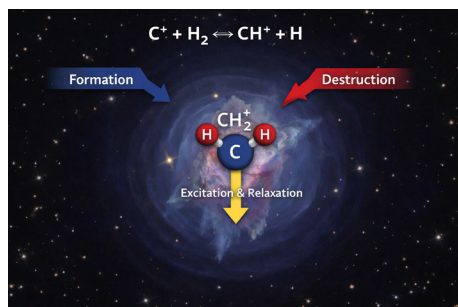
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### Influence of solid helium on the luminescence of nitrogen–neon nanoclusters

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

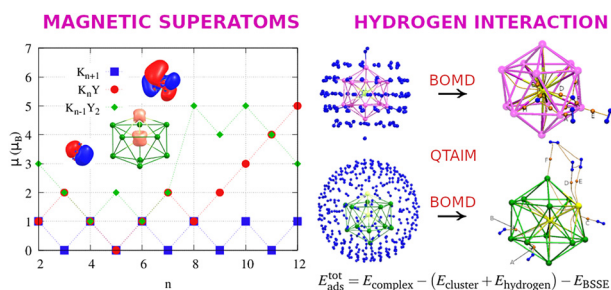
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### Rate constants for a reactive system of astrophysical interest: a statistical study of $CH_2^+$

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

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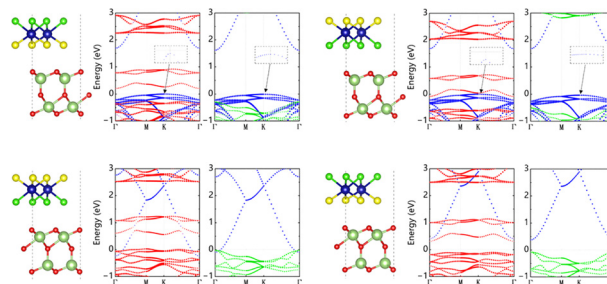


## RESEARCH PAPERS

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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

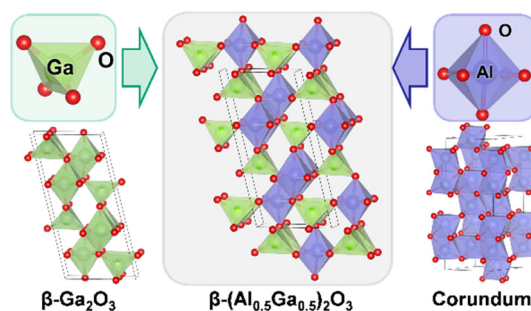
Jing-Jing He, Jun-Yi Gu, Qin-Yue Cao, Ling-Xiao Liu, Min Hua, Jia-Ren Yuan,\* Yan-Dong Guo\* and Xiao-Hong Yan\*



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

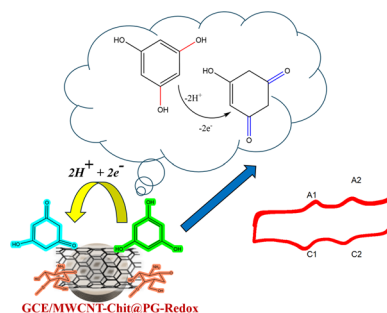
Ziqian Sheng, Wenjing Xu, Xiaoqing Zhou, Cien Liu, Alexander Polyakov, Zhilai Fang, Ning Jia,\* Xiangyu Xu\* and Kelvin H. L. Zhang\*



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

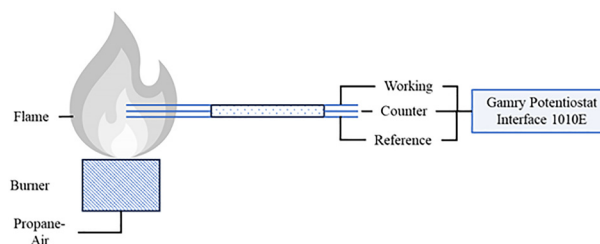
Mansi Gandhi and Anitha Varghese\*



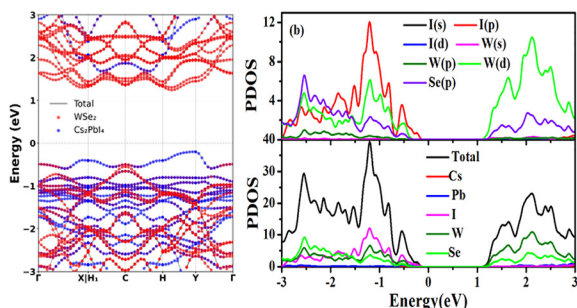
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### Electrochemistry in flame plasmas: passive films and impedance analysis

Bill Logan Riehl\* and Craig E. Banks



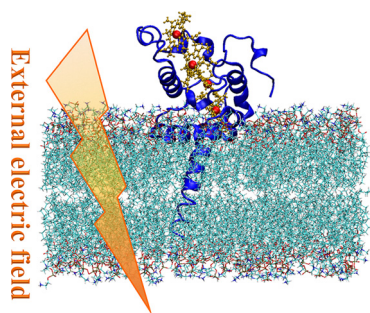
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### Insight into the photoelectric characteristics and photocatalytic water splitting performances of van der Waals heterostructures $\text{Cs}_2\text{PbI}_4/\text{MX}_2$ ( $\text{M} = \text{Mo}, \text{W}$ ; $\text{X} = \text{Se}, \text{S}$ )

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

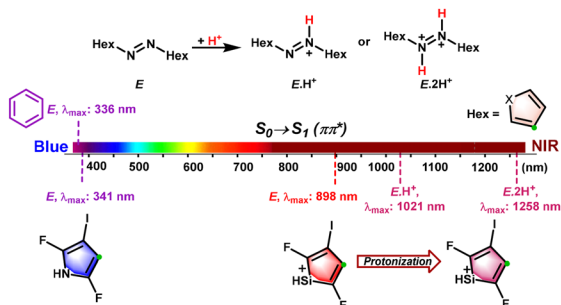
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### Electrostatic and proton–electron interaction in membrane-bound charge transfer proteins under external electric fields: a computational study

Zeinab Rahimi, Amir Lohrasebi\* and Thorsten Koslowski

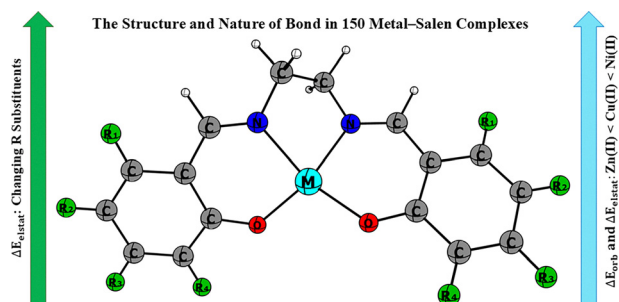
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### Probing the longest $\lambda_{\text{max}}$ of azo compounds in near infrared absorption via integrating protonation, antiaromaticity and substituents: a combined DFT and machine learning study

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

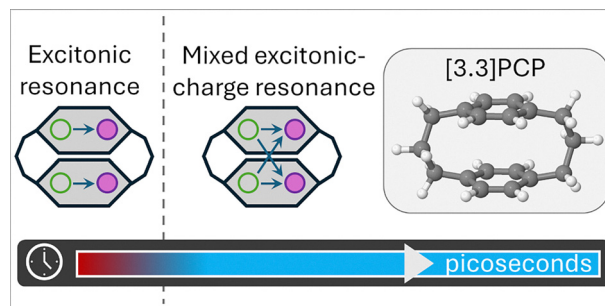
Seyedeh Aghigh Hamrahian, Samaneh Sanei Movafagh and Sadegh Salehzadeh\*



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

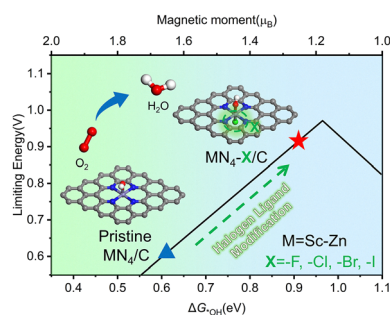
Muhammad Tahir Hafeez, Rafael S. Mattos, Lea M. Ibele\* and Mario Barbatti\*



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

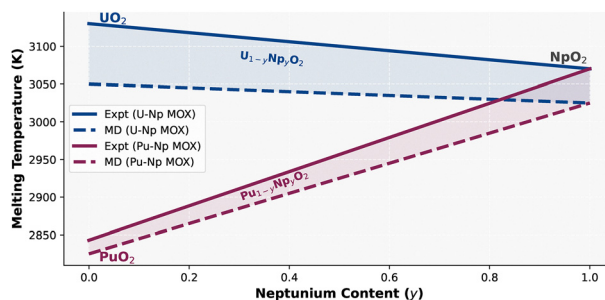
Bo-Yang Luo, Chen Li, Yu-Mei Yang, Wei Du and Ya-Min Wang\*



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

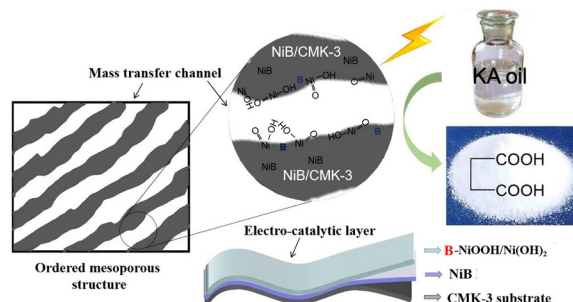
A. Chakraborty, N. Choudhury\* and P. S. Ghosh\*



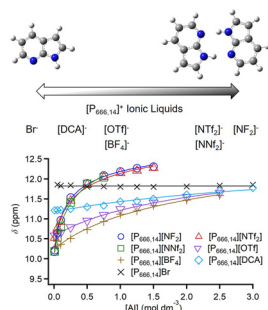
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### Amorphous NiB as an electrocatalyst: from KA oil to succinic acid

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



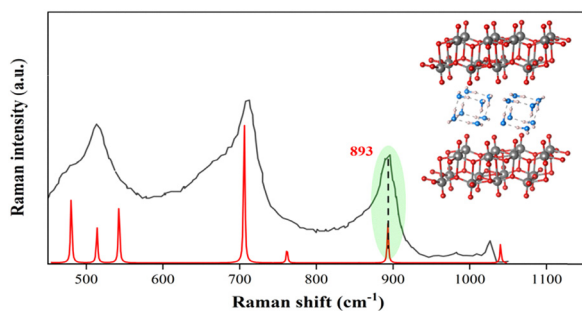
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### Dimer formation of 7-azaindole in phosphonium-based ionic liquids: anion-dependent behavior

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

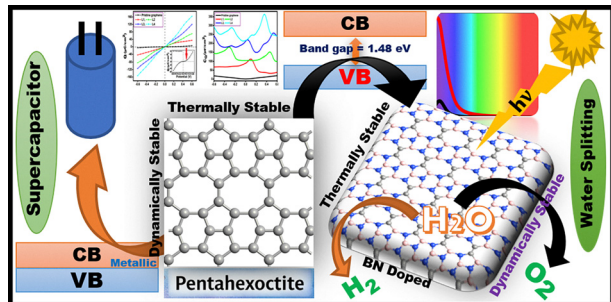
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### A comparative theoretical study on the vibrational spectra of $V_2O_5 \cdot nH_2O$

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

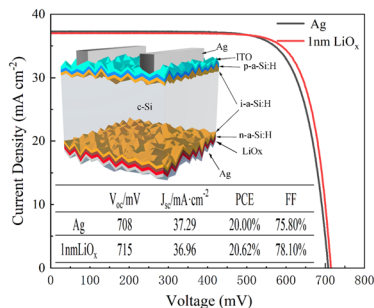
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### Theoretical insights into the structural, electronic, photocatalytic and supercapacitor applications of pentahexoctite

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

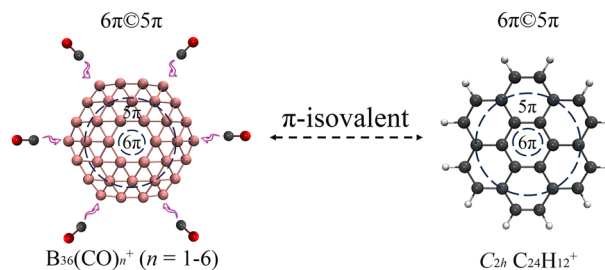
Yusen Lin, Zhi Xu, Zhenjia Wang, Xuanfei Kuang, Yao Xiao, Zijing Wang, Xipeng Zhang and Zongcun Liang\*



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

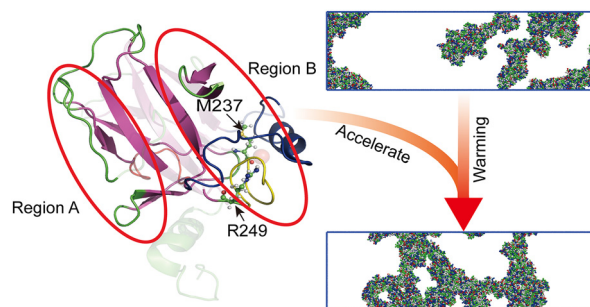
Hong Niu, Qiang Chen,\* Qin-Wei Zhang, Xi Chen, Teng Li, Xiao-Ni Zhao and Si-Dian Li\*



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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

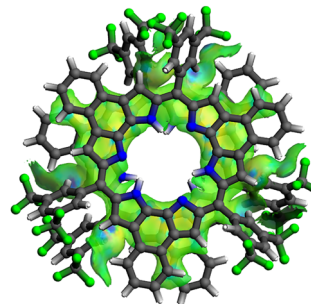
Zhifa Duan, Yi Song, Huanhuan Ruan, Tianjing Guo and Jiangtao Lei\*



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### Insights into the intermolecular interactions between stacked antiaromatic 24- $\pi$ hexaphyrin macrocycles: variation of the magnetic response properties

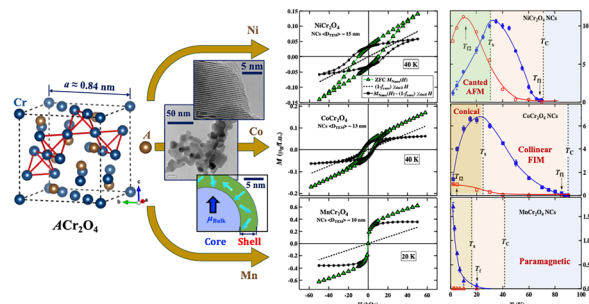
Alvaro Muñoz-Castro



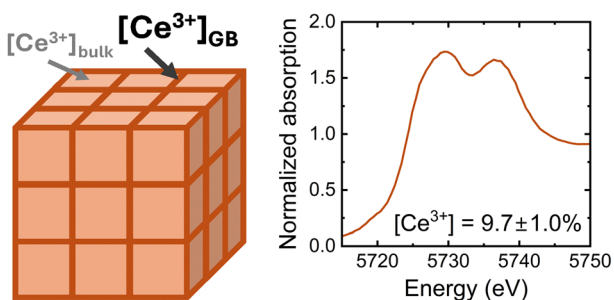
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### Structural, optical, and magnetic properties with finite-size and interface effects of noncollinear ferrimagnetic $ACr_2O_4$ ( $A = Ni, Co,$ and $Mn$ ) single-domain nanocrystals

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



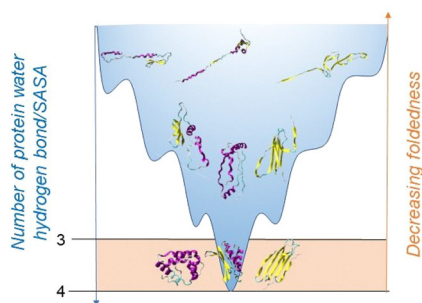
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### Direct *in situ* detection of grain boundary reduction in nanocrystalline ceria

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

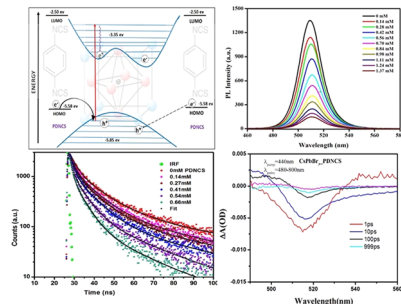
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### Solvent accessible surface area normalized protein–water hydrogen bonds define protein folded state stability and amyloid formation

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

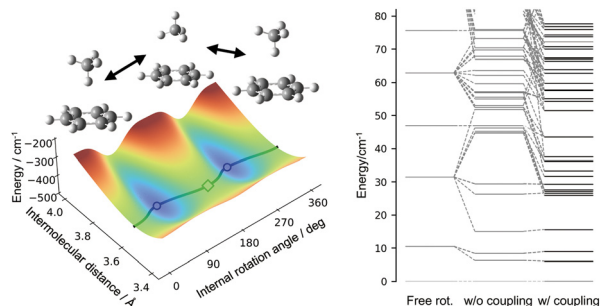
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### Hole transfer dynamics between CsPbBr<sub>3</sub> PNCs and *p*-phenylene diisothiocyanate

Sourav Mandal, Subhadip Giri, Suraj Barman, Sourav Nandi, Shashanka Shekhar Samanta, Sayan Prodhon, 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\*

