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See Ralph A. Wheeler and Emily E. Dalbey, pp. 4593–4602.
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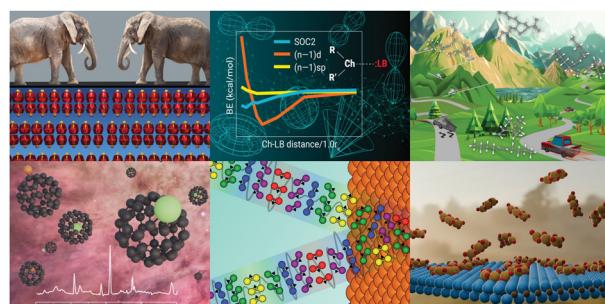
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4514

Physical Chemistry Chemical Physics profiles: contributors to the 2024 Emerging Investigators collection

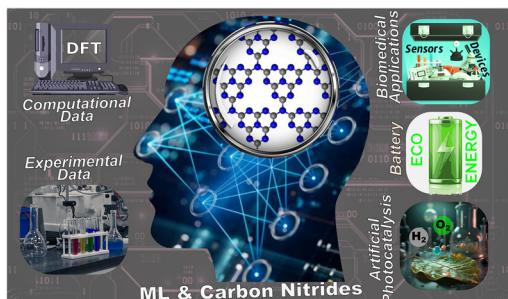


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Navigating the evolution of two-dimensional carbon nitride research: integrating machine learning into conventional approaches

Deep Mondal, Sujoy Datta* and Debnarayan Jana*



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Elemental answers

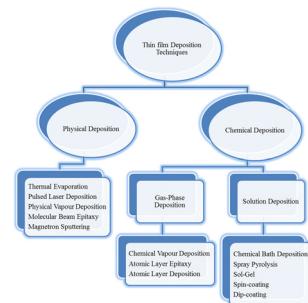
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Review on the optical and electrical properties of chalcogenide thin films: challenges and applications

W. A. Abd El-Ghany

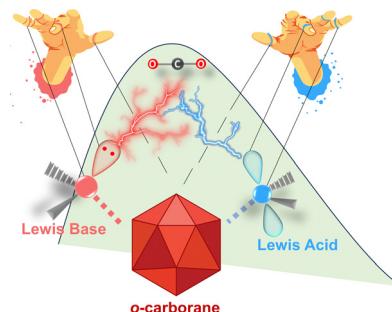


COMMUNICATION

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Puppeteering the reactivity of frustrated Lewis pairs toward CO₂ via coordination dichotomy in bridging units

Mohmmad Faizan and Ravinder Pawar*

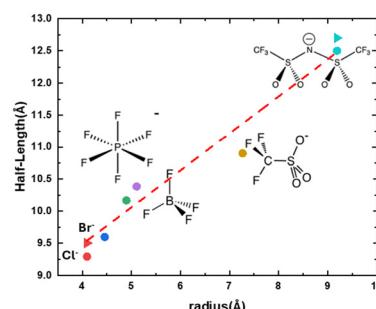


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Structure factor line shape model gives approximate nanoscale size of polar aggregates in pyrrolidinium-based ionic liquids

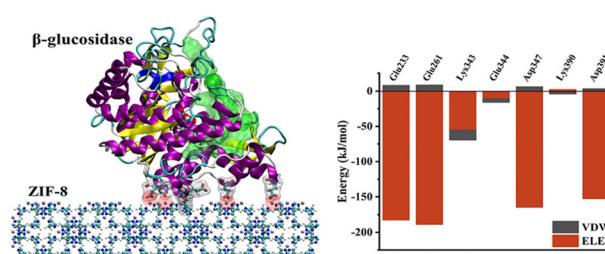
Ralph A. Wheeler* and Emily E. Dalbey



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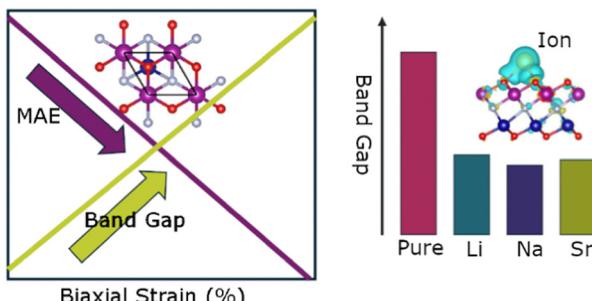
Unraveling the orientation of an enzyme adsorbed onto a metal–organic framework

Zhiyong Xu and Jian Zhou*



RESEARCH PAPERS

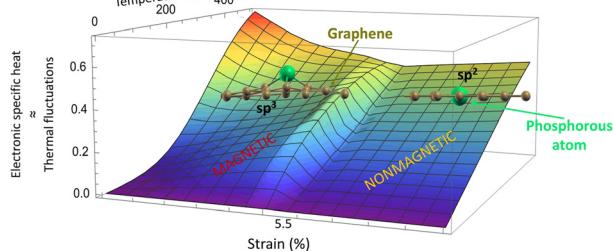
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Modulation of the electronic and magnetic properties of an MnCrNO_2 ferromagnetic semiconductor MXene

Sudil Sandeepa Dewamuni, Buddi Oshada Vithanage, Deniz Çakır and Edirisuriya M. Dilanga Siriwardane*

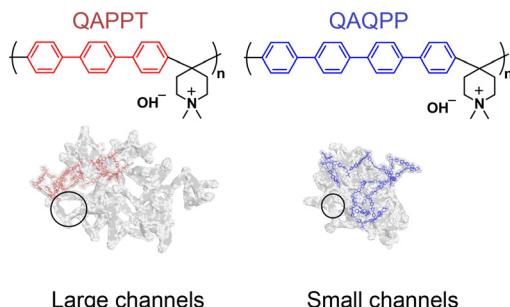
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Magnetic quantum phase transition extension in strained P-doped graphene

Natalia Cortés,* J. Hernández-Tecorralco, L. Meza-Montes, R. de Coss and Patricio Vargas

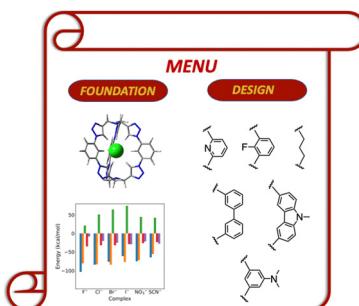
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Atomic insights into the ion-conducting channels of poly(arylene piperidinium) anion exchange membranes

Weiwen Pu and Zhaoru Sun*

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Computer-aided design of triazolo-cages as anion receptors

Minwei Che, Sibali Debnath, Amar H. Flood and Krishnan Raghavachari*

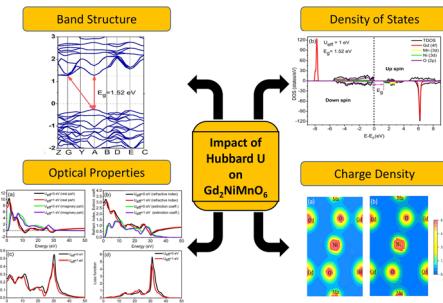


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An *ab initio* approach to investigate the impact of Hubbard *U* correction on the physical properties of $\text{Gd}_2\text{NiMnO}_6$ double perovskite

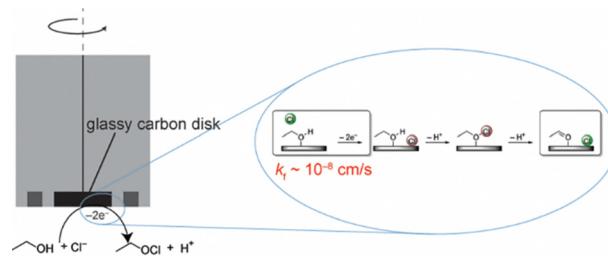
Md. Yasir Arafat, Sweety Akter, Md. Ferdous Shanto, M. J. Hosen* and M. D. I. Bhuyan*



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Insights into the mechanism of electrochemical chloride oxidation in ethanol from X-ray photoelectron spectroscopy, quiescent solution voltammetry, and rotating ring-disk electrodes

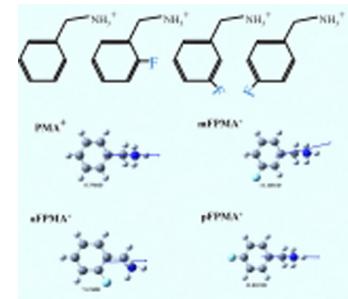
Ryan D. Van Daele, Siqi Li, Katherine H. Morrissey and Bart M. Bartlett*



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Preparation of high-performance quasi-two-dimensional (Q-2D) perovskite solar cells by fluorinated benzylamine groups at different substitution positions

Longtao Du, Jianhua Liao, Kegui Li, Yuge Chang, Qiang Huang, Xiaoyan Gan,* Liling Guo and Hanxing Liu



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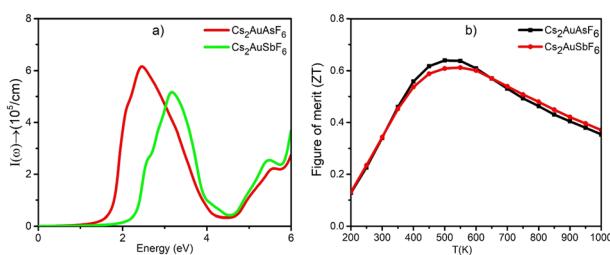
Click and shift: the effect of triazole on solvatochromic dyes

Jean Rouillon,* Carlos Benítez-Martin, Morten Grøtli and Joakim Andréasson*



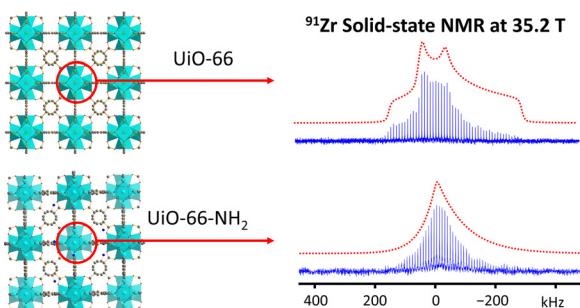
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**Novel $\text{Cs}_2\text{Au}^{\text{I}}\text{M}^{\text{III}}\text{F}_6$ ($\text{M} = \text{As}, \text{Sb}$) double halide perovskites: sunlight and industrial waste heat management device applications**

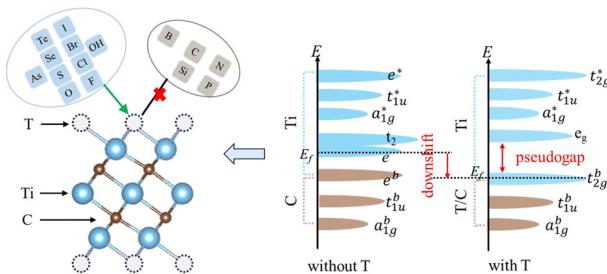
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**Local order, disorder, and everything in between: using ^{91}Zr solid-state NMR spectroscopy to probe zirconium-based metal–organic frameworks**

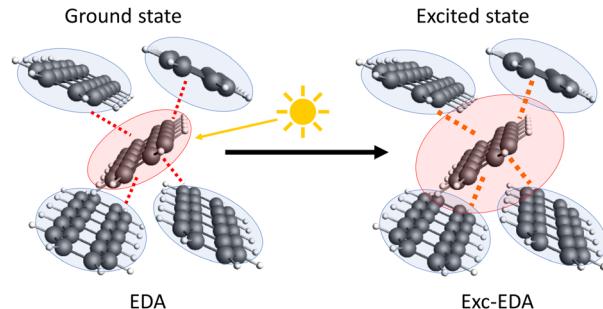
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Meng Tian

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**Energy decomposition analysis for excited states: an extension based on TDDFT**

Florian Kreuter and Ralf Tonner-Zech*

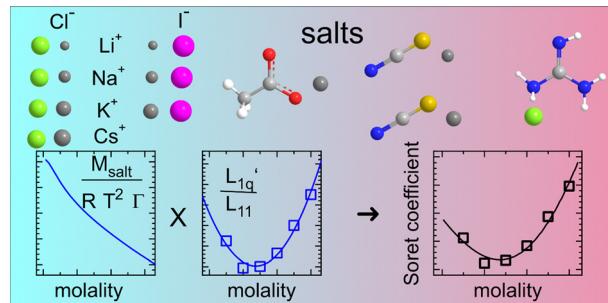


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Analyzing the concentration-dependent Soret coefficient minimum in salt solutions: an overview

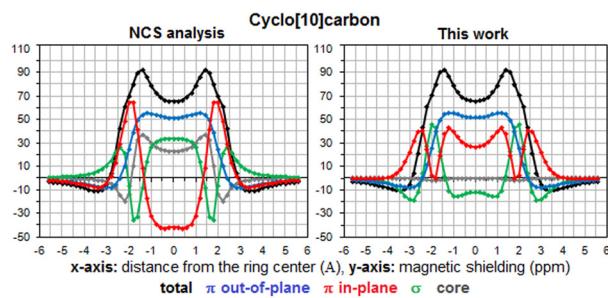
Binny A. Rudani, W. J. Briels* and Simone Wiegand*



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Orbital contributions to the magnetic shielding of cyclo[2n]carbons ($n = 3–12$)

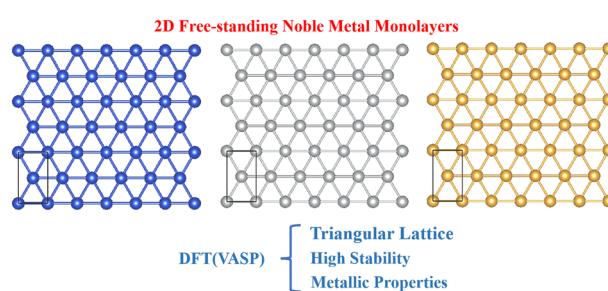
Marija Baranac-Stojanović



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Structure, stability and electronic properties of two-dimensional monolayer noble metals with triangular lattices: Cu, Ag, and Au

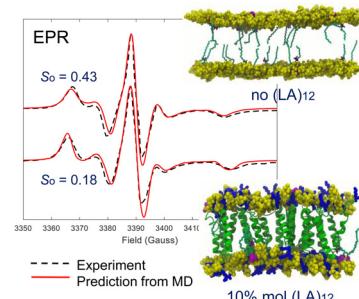
Zhefeng Wang, Kai Chen, Youmin Xu, Zengjie Wang, Lingbao Kong, Songyou Wang* and Wan-Sheng Su*



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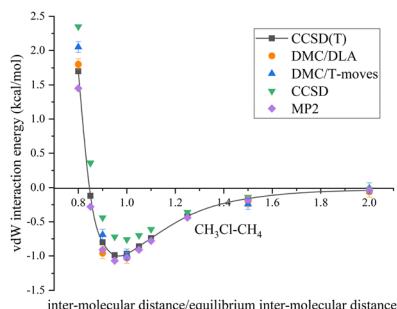
Predicting and interpreting EPR spectra of POPC lipid bilayers with transmembrane α -helical peptides from all-atom molecular dynamics simulations

Andrea Catte and Vasily S. Oganesyan*



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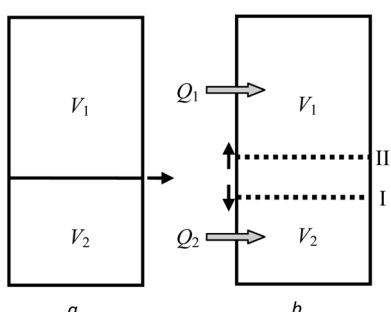
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Accuracy of the diffusion quantum Monte Carlo method on dissociation curves of van der Waals systems with the single-Slater–Jastrow trial wavefunction

Zhiru Huang, Xiaojun Zhou and Fan Wang*

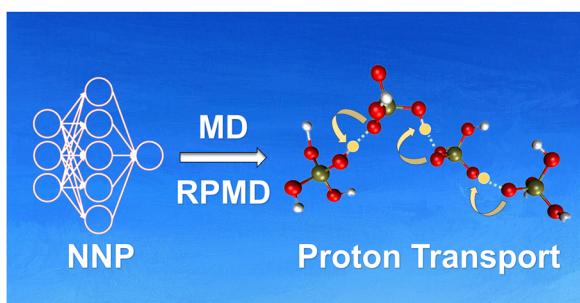
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Mixing of real and quantum gases

Andrey Ya. Borshchevskii*

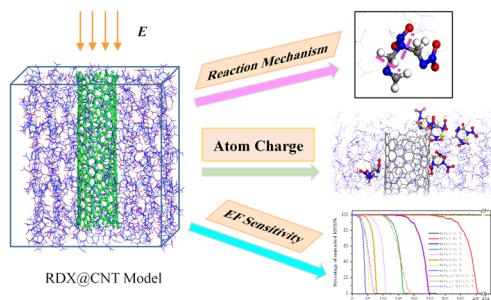
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Proton transport in liquid phosphoric acid: the role of nuclear quantum effects revealed by neural network potential

Pei Liu, Wei Li* and Shuhua Li*

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Reaction mechanism and sensitivity enhancement of energetic materials doped with carbon nanotubes under electric fields by molecular dynamics simulations

Junjian Li, Junying Wu,* Yiping Shang, Yule Yao, Ruizheng Liu, Jianyu Wang and Lang Chen

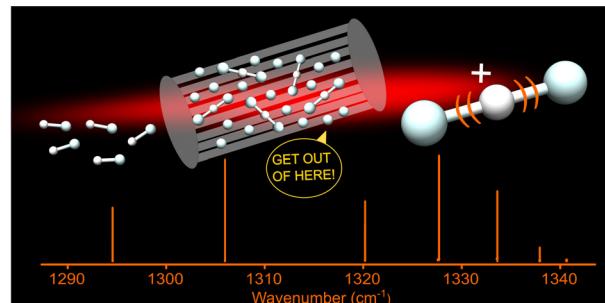


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High-resolution leak-out spectroscopy of HHe₂⁺

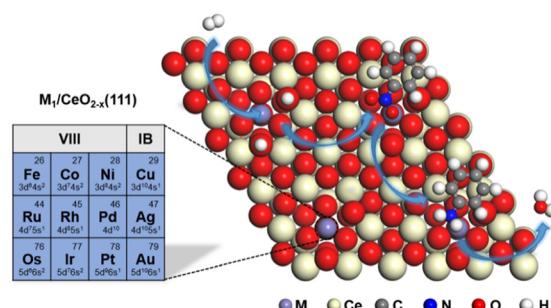
Thomas Salomon, Carlo Baddeliyanage, Carla Schladt, Irén Simkó, Attila G. Császár, Wesley G. D. P. Silva, Stephan Schlemmer and Oskar Asvany*



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Theoretical study on nitrobenzene hydrogenation to aniline catalyzed by M₁/CeO_{2-x}(111) single-atom catalysts

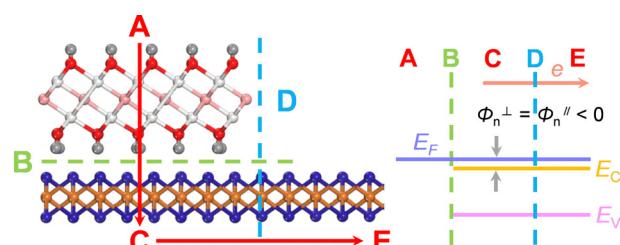
Haohao Wang, Min Pu and Ming Lei*



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Functionalized Sc₂N as Ohmic-contact electrodes for monolayer PtSe₂: an *ab initio* study

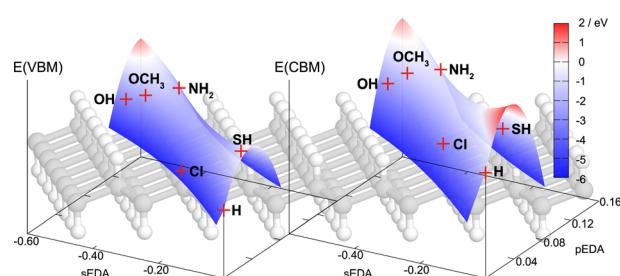
Hong Li,* Jiahui Li, Chaoyang Fan, Fengbin Liu, Shuai Sun and Jing Lu*



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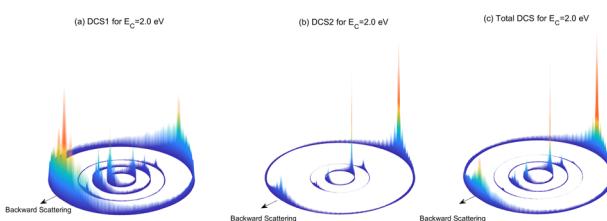
Ligand impacts on band edge energies and excited state splittings of silicane

Guoying Yao, Ekadashi Pradhan, Zhenyu Yang* and Tao Zeng*



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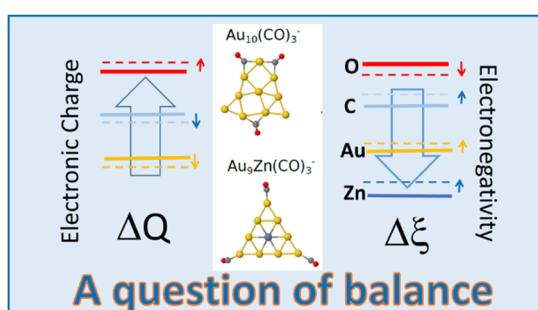
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Quantum state-to-state dynamics of C(³P) + H₂(X¹Σ_g⁺) → CH(²Π) + H(²S) reaction based on a new CH₂ (X³A'') potential energy surface

Juan Zhao, Daguang Yue, Dong Liu, Shang Gao, Lifei Wang and Lulu Zhang*

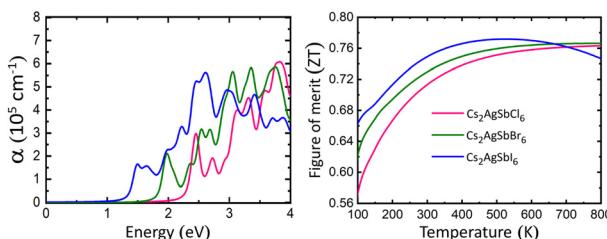
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Sequential adsorption of multiple CO molecules on Au₁₀⁻ and Au₉Zn⁻ triangular clusters: the crucial role of a single atomic impurity

Eva M. Fernández* and Luis C. Balbás

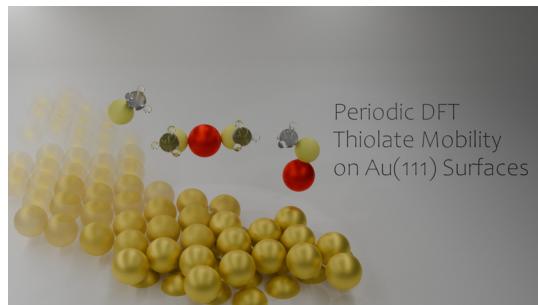
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Exploring double perovskites Cs₂AgSbX₆ (X = Cl, Br, and I) as promising optoelectronic and thermoelectric materials: a first-principles study

Asim Sajjad, Muhammad Faizan,* Tahani A. Alrebdī, Ghulam Murtaza, Javed Rehman, Xingchen Shen, Yujing Dong, Kausar Shaheen and Shah Haidar Khan*

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Mobility of thiolates on Au(111) surfaces

Daniël R. Duijnstee, Moniek Tromp, Wesley R. Browne* and Aleksandar Staykov*

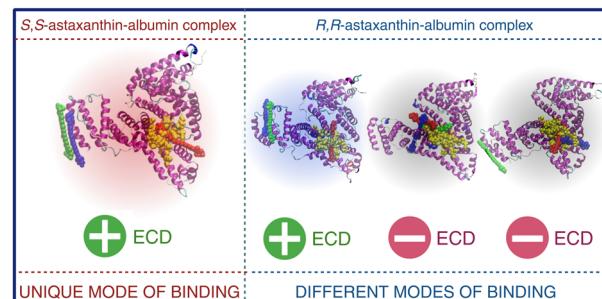


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Enantiorecognition in a multi-component environment

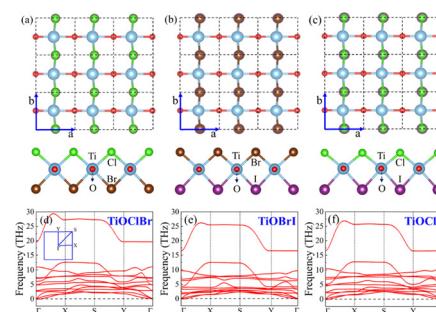
Joanna Mazurkiewicz, Ewa Staneck, Pedro Maximiano, Tiago H. Ferreira, Marta Karpiel, Szymon Buda, Justyna Kalinowska-Tłuszcik, Pedro N. Simões, Igor Reva and Agnieszka Kaczor*



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Prediction of two-dimensional narrow-gap Janus TiO_XY (X, Y = Cl, Br, I; X ≠ Y) monolayers for electronic and optoelectronic applications

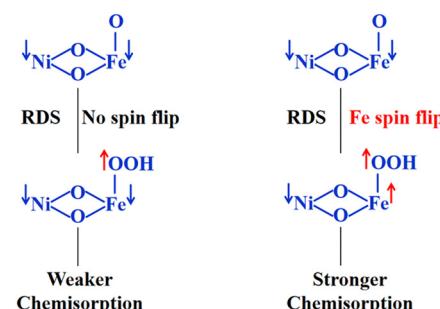
Yange Peng, Xiuwen Wu, Shengzhao Yang, Jiansheng Dong, Xi Fu, Hairui Bao* and Wenhua Liao*



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Oxygen evolution reaction on NiFe-LDH/(Ni,Fe)OOH: theoretical insights into the effects of electronic structure and spin-state evolution

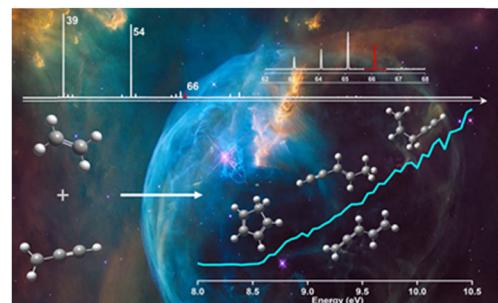
Qian Lin, Guangjun Nan, Dawei Fu and Liyan Xie*



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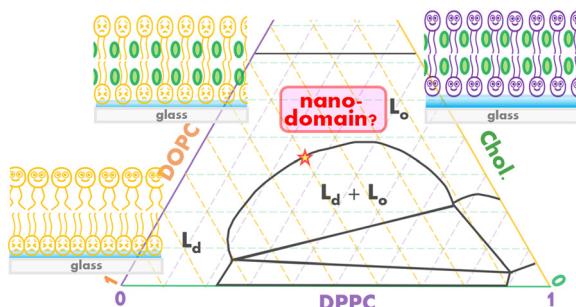
Formation of C₅H₆ isomers: a combination of experimental and computational investigation

Yi-Fan Zhang, Wang Li,* Chang-Yang Wang, Chen Huang, Hui-Ting Bian* and Long Zhao*



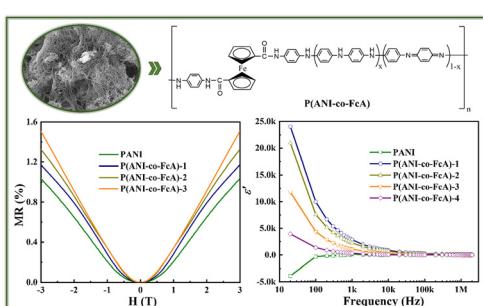
RESEARCH PAPERS

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**A macroscopically homogeneous lipid phase exhibits leaflet-specific lipid diffusion in a glass-supported lipid bilayer**

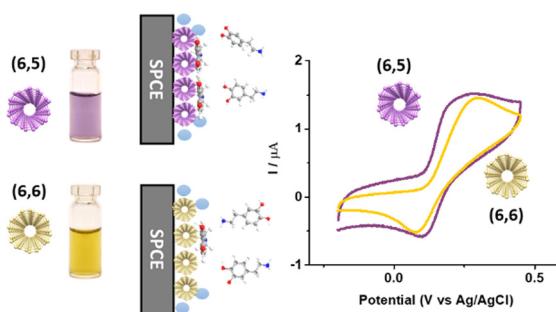
Takuhiko Otosu,* Miyuki Sakaguchi and Shoichi Yamaguchi

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**Ferrocene derivatives and aniline copolymers with tunable magnetoresistance and dielectric properties**

Huiyan Ren and Hongbo Gu*

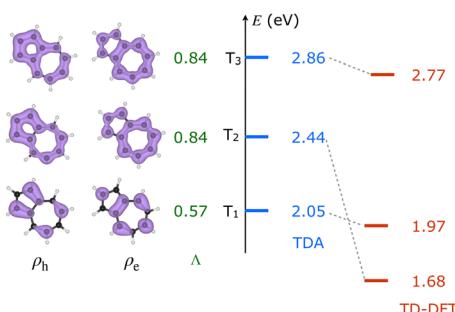
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**Single-chirality single-wall carbon nanotubes for electrochemical biosensing**

Ju-Yeon Seo, Bahar Mostafiz, Xiaomin Tu, Constantine Y. Khripin, Ming Zheng, Han Li* and Emilia Peltola*

COMMENTS

4968

**Comment on “Designing potentially singlet fission materials with an anti-Kasha behaviour” by R. Pino-Rios, R. Báez-Grez, D. W. Szczepanik, and M. Solá, *Phys. Chem. Chem. Phys.*, 2024, 26, 15386**

Komal Jindal, Atreyee Majumdar and Raghunathan Ramakrishnan*

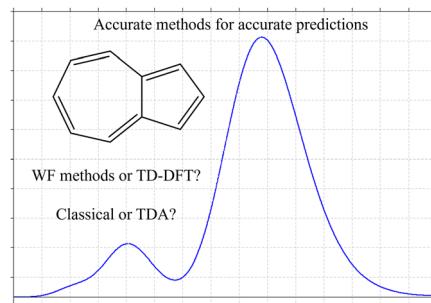


COMMENTS

4973

Reply to the 'Comment on "Designing potentially singlet fission materials with an anti-Kasha behaviour" by K. Jindal, A. Majumdar and R. Ramakrishnan, *Phys. Chem. Chem. Phys.*, 2025, 27, DOI: 10.1039/D4CP02863E

Ricardo Pino-Rios,* Rodrigo Báez-Grez,
Dariusz W. Szczepanik and Miquel Solà*



CORRECTION

4976

Correction: Designing potentially singlet fission materials with an anti-Kasha behaviour

Ricardo Pino-Rios,* Rodrigo Báez-Grez, Dariusz W. Szczepanik and Miquel Solà*