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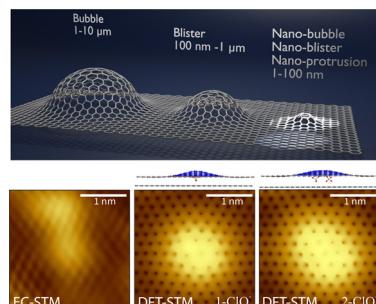
See Hussam Bouaamlat,
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Nano-protrusions in intercalated graphite: understanding the structural and electronic effects through DFT

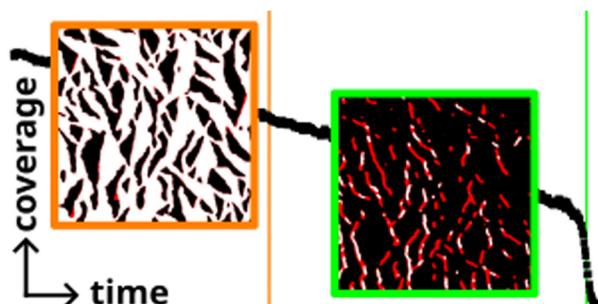
Hussam Bouaamlat,* Ari Paavo Seitsonen,
Gianlorenzo Bussetti, Rossella Yivlialin, Stefania De Rosa,
Paolo Branchini and Luca Tortora*



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Impact of long-range attraction on desorption kinetics

Florian Schneider,* Lukas Höltkemeier, Andrea Floris,
Lev Kantorovich, Ralf Bechstein and Angelika Kühnle*





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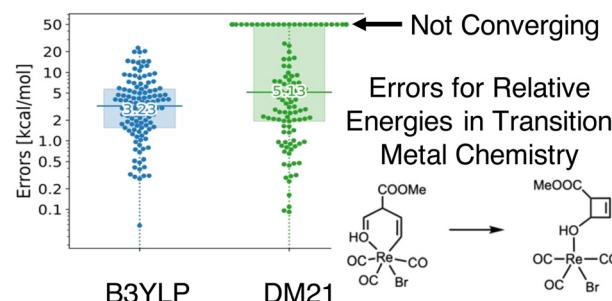
Fundamental questions
Elemental answers

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Deep Mind 21 functional does not extrapolate to transition metal chemistry

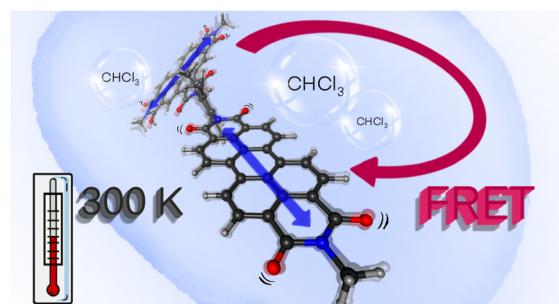
Heng Zhao, Tim Gould and Stefan Vuckovic*



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Resonance energy transfer in orthogonally arranged chromophores: a question of molecular representation

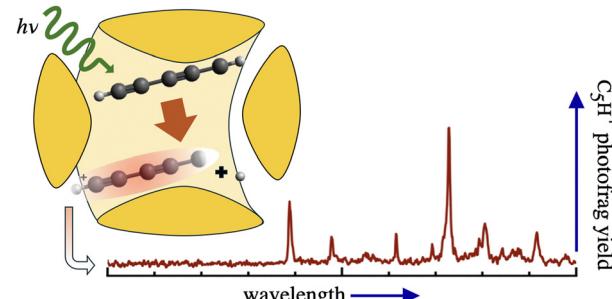
Richard Jacobi and Leticia González*



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Gas-phase electronic spectra of $\text{HC}_{2n+1}\text{H}^+$ ($n = 2\text{--}6$) chains

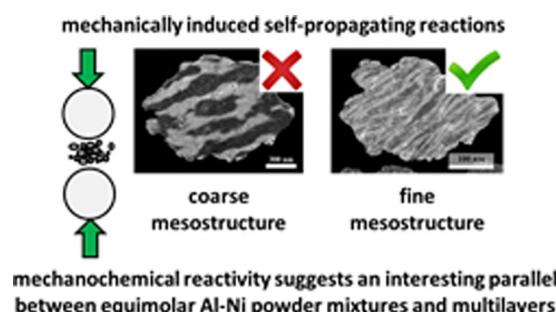
Samuel J. P. Marlton, Chang Liu, Patrick Watkins and Evan J. Bieske*



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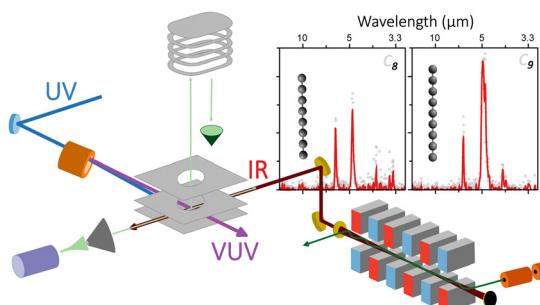
Mechanochemical ignition of self-propagating reactions in equimolar Al–Ni powder mixtures and multilayers

Maria Carta and Francesco Delogu*



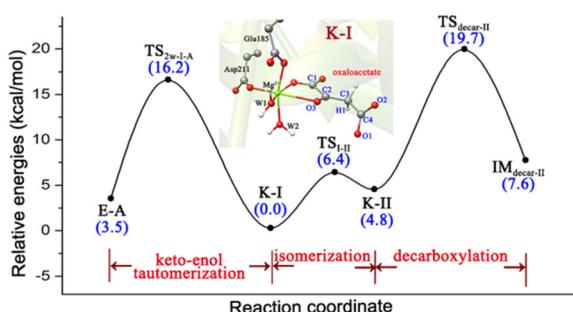
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**Infrared bands of neutral gas-phase carbon clusters in a broad spectral range**

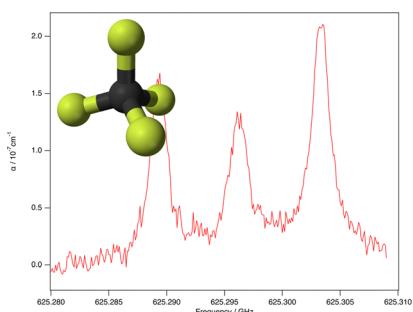
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**Computational insights into the binding modes, keto-enol tautomerization and stereo-electronically controlled decarboxylation of oxaloacetate in the active site of macrophomate synthase**

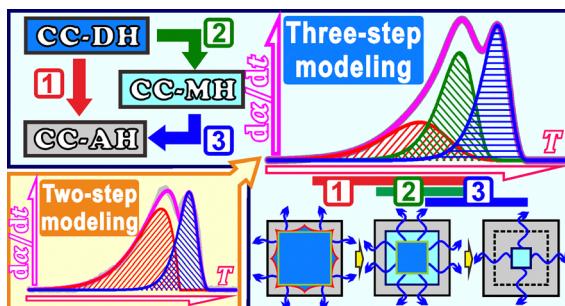
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**The physico-geometrical reaction pathway and kinetics of multistep thermal dehydration of calcium chloride dihydrate in a dry nitrogen stream**

Kazuki Kato and Nobuyoshi Koga*

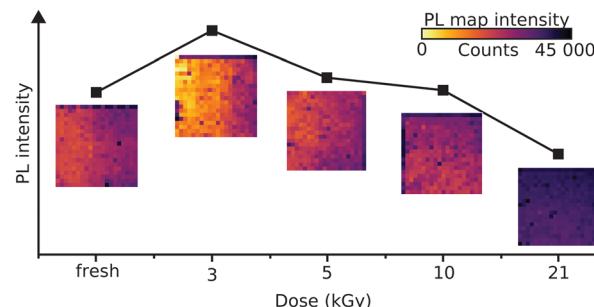


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Gamma-ray dose threshold for MAPbI₃ solar cells

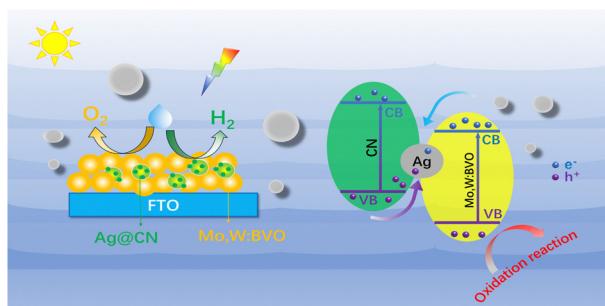
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Synergistic effect of Ag@CN with BiVO₄ in a unique Z-type heterojunction for enhancing photoelectrochemical water splitting performance

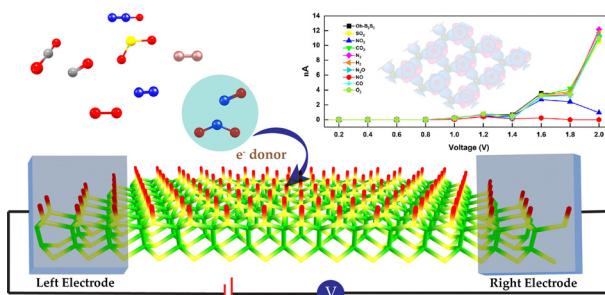
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Realization of efficient and selective NO and NO₂ detection via surface functionalized h-B₂S₂ monolayer

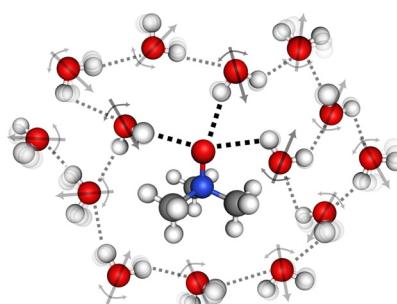
Upasana Nath and Manabendra Sarma*



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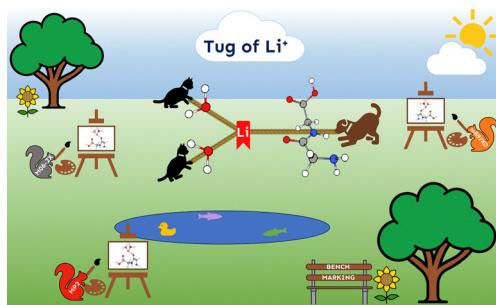
TMAO perturbs intermolecular vibrational motions of water revealed by low-frequency modes

Tsung-Han Liu and Masanari Okuno*



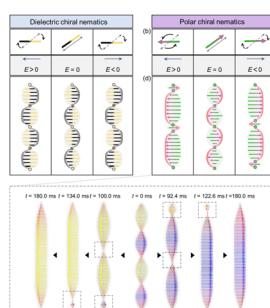
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**The impact of solvation on the structure and electric field strength in Li⁺GlyGly complexes**

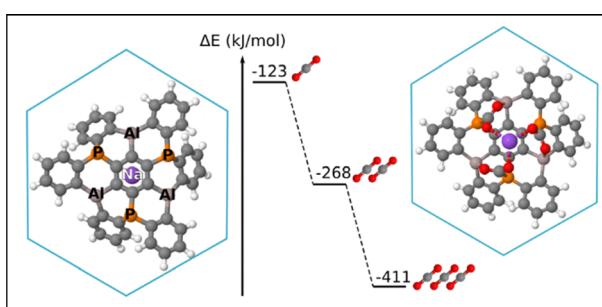
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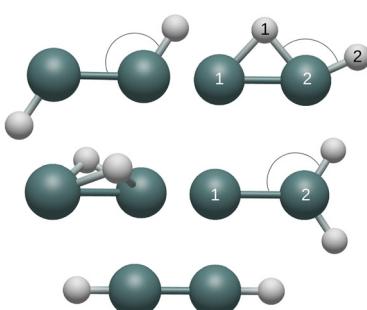
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Ethan J. Poncelet, Henry F. Mull, Yohannes Abate, Gregory H. Robinson, Gary E. Doublerly, Justin M. Turney and Henry F. Shaefer III

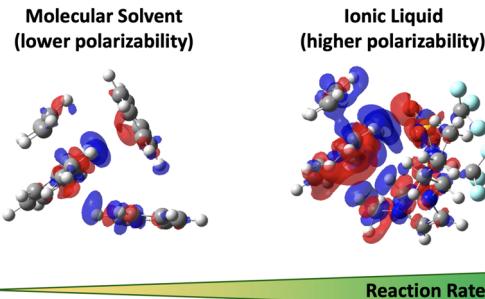


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Unravelling ionic liquid solvent effects for a non-polar Cope rearrangement reaction

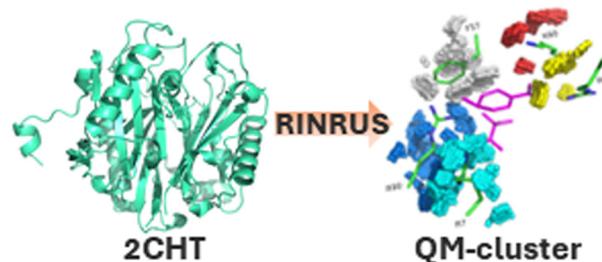
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The influence of model building schemes and molecular dynamics sampling on QM-cluster models: the chorismate mutase case study

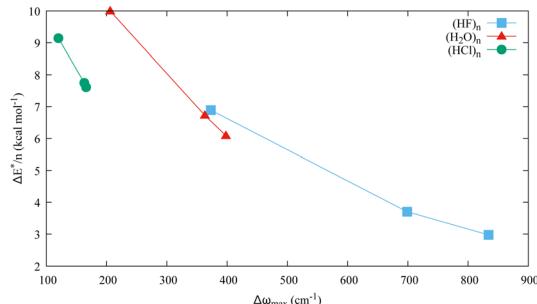
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Systematic analysis of electronic barrier heights and widths for concerted proton transfer in cyclic hydrogen bonded clusters: $(HF)_n$, $(HCl)_n$ and $(H_2O)_n$ where $n = 3, 4, 5$

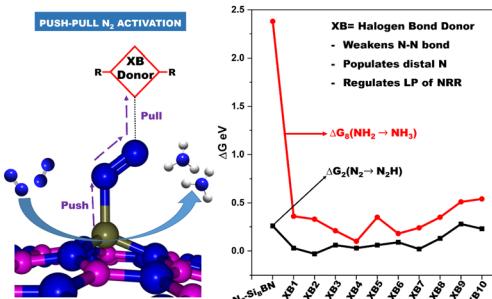
Yuan Xue, Thomas More Sexton, Johnny Yang and Gregory S. Tschumper*



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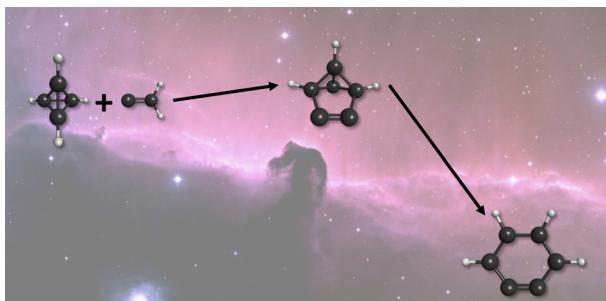
Harnessing halogen bond donors for enhanced nitrogen reduction: a case study on metal-free boron nitride single-atom catalysts

Venkata Surya Kumar Choutipalli* and Venkatesan Subramanian*



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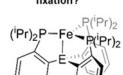
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**Bridging the gap: viable reaction pathways from tetrahedrane to benzyne**

Taylor A. Cole, Steven R. Davis, Athena R. Flint and Ryan C. Fortenberry*

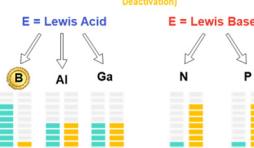
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What is the best anchor atom for biomimetic nitrogen fixation?



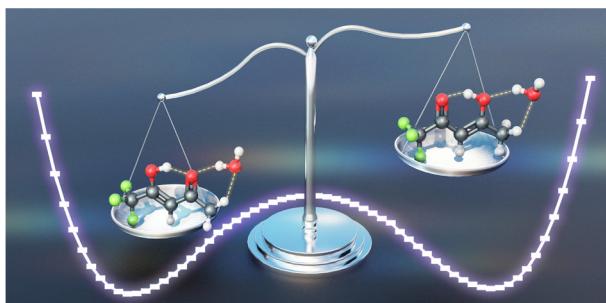
Ease of Catalyst Regeneration

HER Side Reactions (Catalyst Deactivation)

**Role of Lewis acid/base anchor atoms in catalyst regeneration: a comprehensive study on biomimetic EP_3Fe nitrogenases**

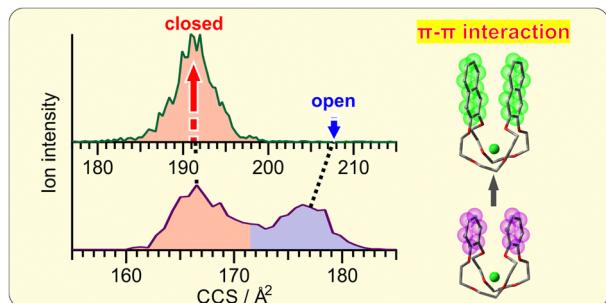
Joseph Kfoury and Julianna Oláh*

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**A rotational spectroscopy study of microsolvation effects on intramolecular proton transfer in trifluoroacetylacetone–(H_2O)_{1–3}**

Dingding Lv, Xinlei Chen, Ningjing Jiang, Guanjun Wang, Xiaoqing Zeng, Wei Fang,* Weixing Li* and Mingfei Zhou*

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**Intra-host $\pi-\pi$ interactions in crown ether complexes revealed by cryogenic ion mobility-mass spectrometry**

Ryosuke Ito, Keijiro Ohshima* and Fuminori Misaizu*

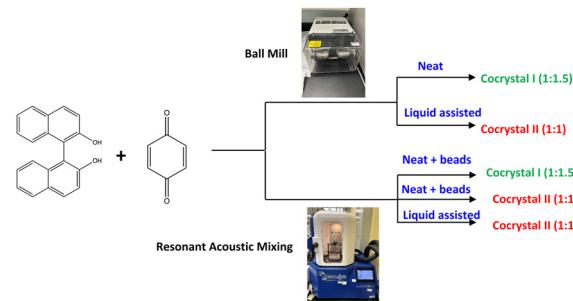


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Comparison of mechanochemical methods in the synthesis of binaphthol–benzoquinone based cocrystals

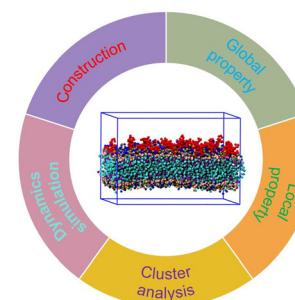
Siddarth Nagapudi and Karthik Nagapudi*



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Effect of GM1 concentration change on plasma membrane: molecular dynamics simulation and analysis

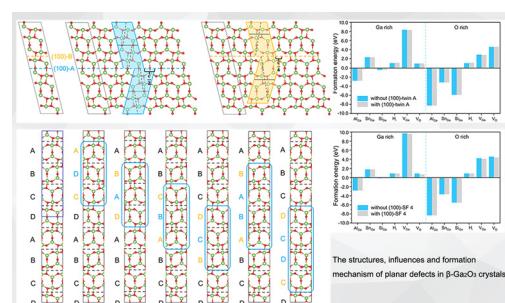
Yongkang Lyu, Shuo Chen, Yu Zhao, Hongxiu Yuan, Chenyang Zhang, Changzhe Zhang and Qingtian Meng*



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Structures, influences, and formation mechanism of planar defects on (100), (001) and (−201) planes in β -Ga₂O₃ crystals

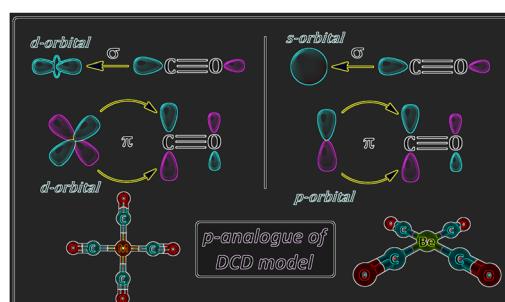
Qi Li, Xin Guan, Yu Zhong, Zhitai Jia,* Yang Li* and Na Lin*



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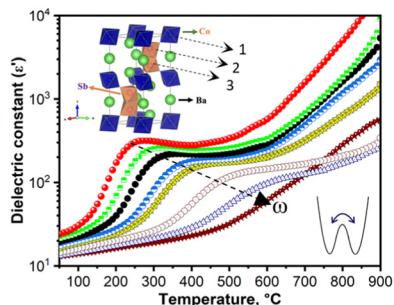
Beryllium carbonyl Be(CO)_n ($n = 1\text{--}4$) complex: a p-orbital analogy of Dewar–Chatt–Duncanson model

Siddhartha K. Purkayastha, Shahnaz S. Rohman, Pattiyl Parameswaran* and Ankur K. Guha*



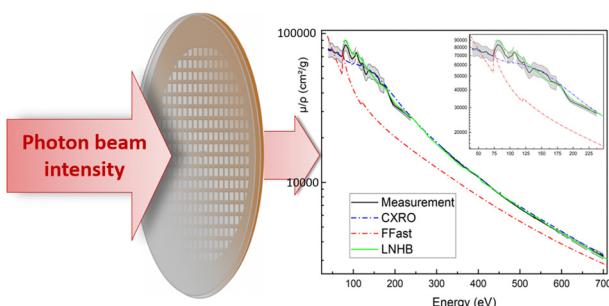
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**Relaxor ferroelectric-like glassy dielectric dispersion in the triple perovskite $\text{Ba}_3\text{CoSb}_2\text{O}_9$**

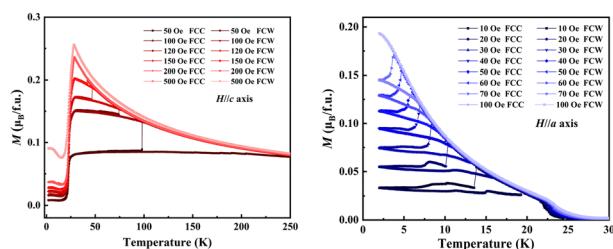
Sanjay Kumar, Rashi Nathawat,* Arvind Kumar Yogi and Satyapal S. Rathore

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**High-accuracy experimental determination of photon mass attenuation coefficients of transition metals and lithium fluoride in the ultra-soft energy range**

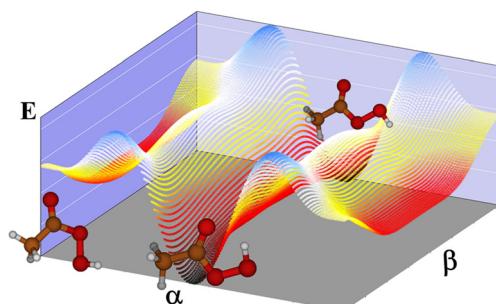
Pia Schweizer,* Yves Ménesguen, Marie-Christine Lépy, Emmanuelle Brackx, Maxime Duchateau and Philippe Jonnard

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**Low field controllable continuous spin switching in the thulium–ytterbium single crystal**

Wencheng Fan, Xiaoxuan Ma, Gang Zhao, Haiyang Chen, Rongrong Jia, Baojuan Kang, Zhenjie Feng, Jun-Yi Ge, Jincang Zhang and Shixun Cao*

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**Theoretical structural and spectroscopic characterization of peroxyacetic acid ($\text{CH}_3\text{-CO-OOH}$): study of the far infrared region**

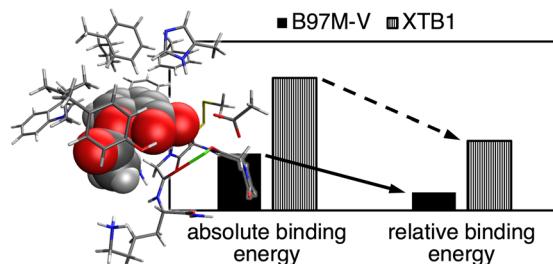
Sinda Brahem, Dorsaf Missaoui, Ounaies Yazidi, Faouzi Najar and María Luisa Senent*

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Sorting drug conformers in enzyme active sites: the XTB way

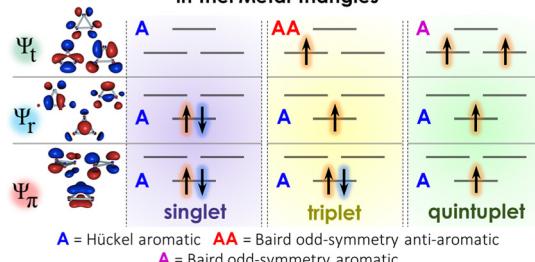
Bun Chan,* William Dawson and Takahito Nakajima

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Unveiling the quantum secrets of triel metal triangles: a tale of stability, aromaticity, and relativistic effects

Silvia Escayola, Elisa Jimenez-Izal, Eduard Matito, Jesus M. Ugalde, Rafael Grande-Aztatzi* and Jose M. Mercero*

Mandado's 2n+1 Rule: Spin Separated Aromaticity in Triel Metal Triangles

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A highly conductive and robust micrometre-sized SiO anode enabled by an *in situ* grown CNT network with a safe petroleum ether carbon source

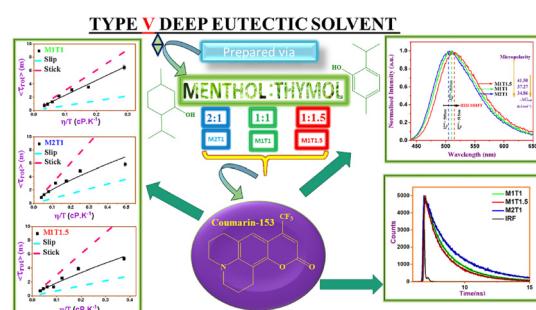
Xiaobo Duan,* Jiaao Yu, Yancai Liu, Yanqiang Lan, Jian Zhou, Birou Lu, Lina Zan, Zimin Fan and Lei Zhang*



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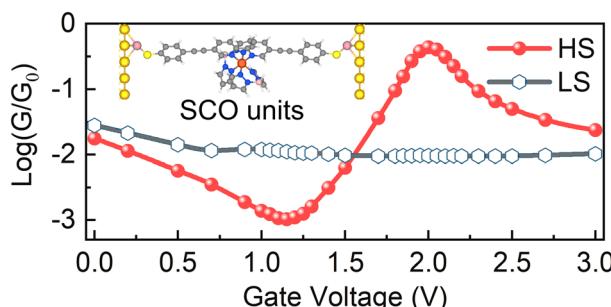
Solute dynamics of a hydrophobic molecule in a menthol–thymol based type-V deep eutectic solvent: effect of composition of the components

Sagar Srivastava, Sapana Sinha, Sanyukta Bhattacharjee and Debabrata Seth*



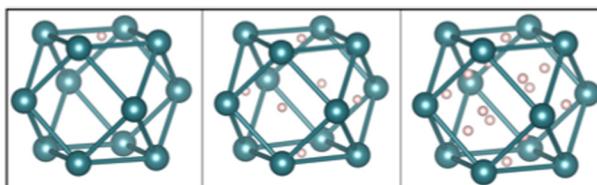
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**Fano resonance in molecular junctions of spin crossover complexes**

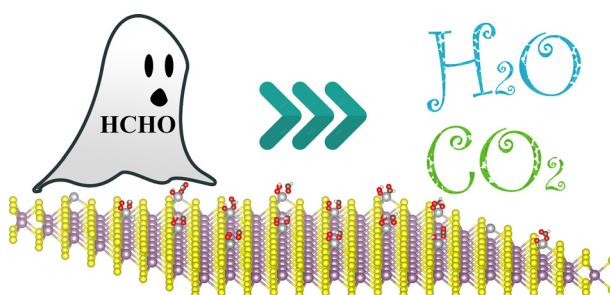
Hua Hao,* Honghao Li, Ting Jia, Yanhong Zhou and Xiaohong Zheng*

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**Electronic structure and thermodynamic approaches to the prospect of super abundant vacancies in δ -Pu**

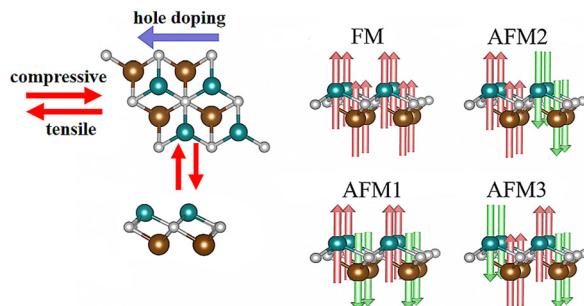
Alexander Muñoz,* Ivana Matanovic, Brendan Gifford, Sven Rudin, Troy Holland and Travis Jones*

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**A first-principles study on Ni-decorated MoS₂ for efficient formaldehyde degradation over a wide temperature range**

Jiahui Tang, Xiaocha Wang, Honggang Pan* and Baozeng Zhou*

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**Tuning the magnetic properties of double transition-metal carbide CoMC (M = Ti, V, Cr, Mn, Fe, Ni) monolayers**

Honghai Zhang, Yaya Lou, Dongni Wu, Yangfang Liao and Jing Xie*

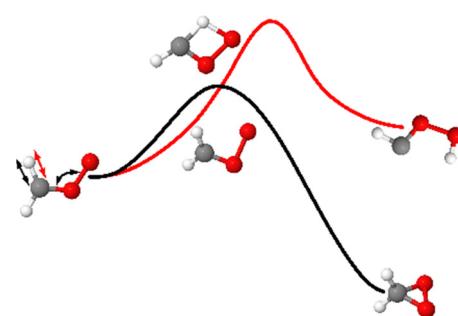


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OH-Formation following vibrationally induced reaction dynamics of H₂COO

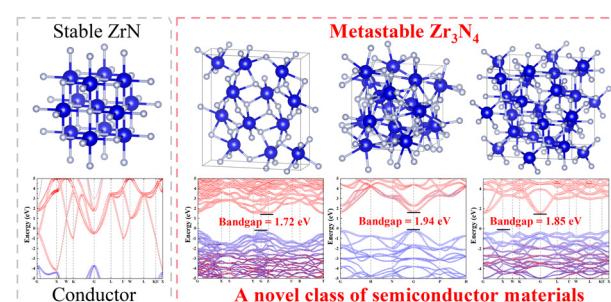
Kaisheng Song, Meenu Upadhyay and Markus Meuwly*



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Electronic and elastic properties of metastable Zr₃N₄: a joint experimental and theoretical study

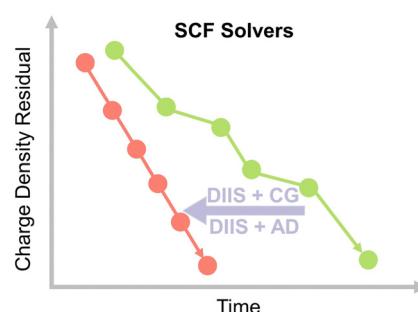
Yuhe Liu, Kunlun Wang, Nina Ge, Hui Sun, Bo Dai and Yong Wang*



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Refining DIIS algorithms for Si and GaAs solar cells: incorporation of weight regularization, conjugate gradient, and reverse automatic differentiation techniques

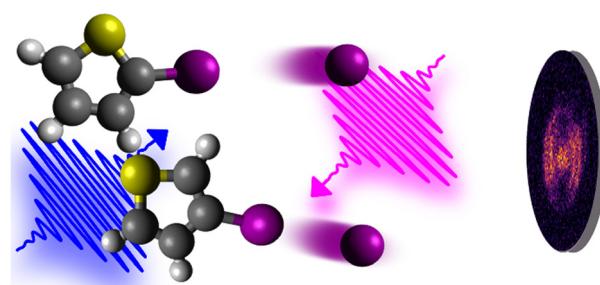
Zhaosheng Zhang,* Sijia Liu and Yingjie Zhang



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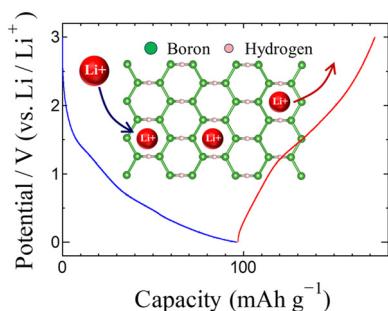
Exploring the ultrafast and isomer-dependent photodissociation of iodothiophenes via site-selective ionization

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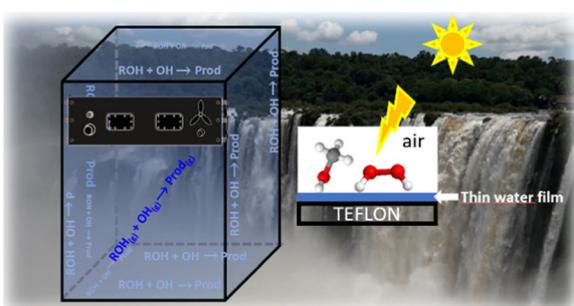
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**Lithium-ion battery electrode properties of hydrogen boride**

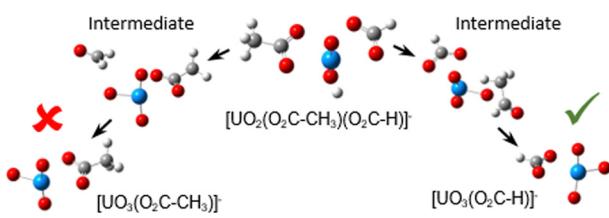
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**Understanding the active role of water in laboratory chamber studies of reactions of the OH radical with alcohols of atmospheric relevance**

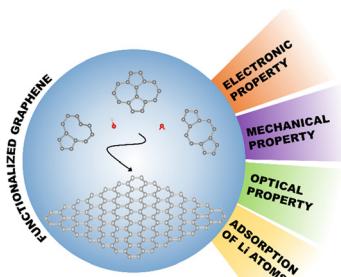
María de los A. Garavagno, Federico J. Hernández, Rafael A. Jara-Toro and Gustavo A. Pino*

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**Reactions of gas-phase uranyl formate/acetate anions: reduction of carboxylate ligands to aldehydes by intra-complex hydride attack**

Amanda R. Bubas, Irena J. Tatosian, Anna Iacovino, Theodore A. Corcovilos and Michael J. van Stipdonk*

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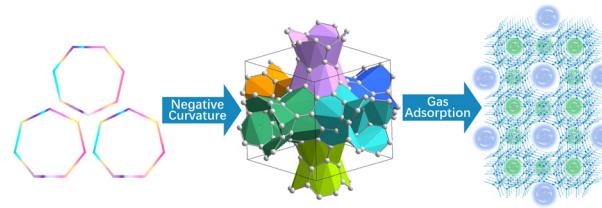
**Distribution of oxygen-containing functional groups on defective graphene: properties engineering and Li adsorption**

Jiang Xiang, Jing Xu, Hongyan Li, Liang Chen and Wei Liu*



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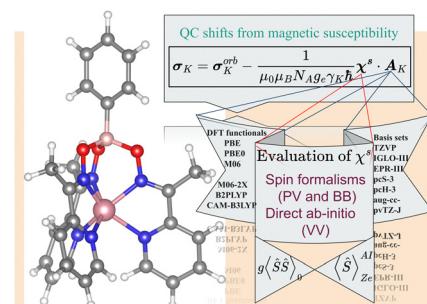
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The smallest Schwarzite carbon with only heptagonal carbon ringsMeng Hu, Junwen Huang, Lu Shi, Jing Hua,*
Lingyu Liu, Julong He and Jianning Ding

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Delving into theoretical and computational considerations for accurate calculation of chemical shifts in paramagnetic transition metal systems using quantum chemical methods

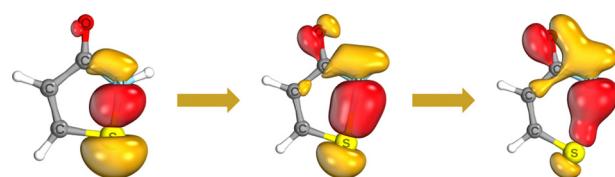
Md. Ashraful Islam* and Andrew J. Pell*



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From skin sensitizers to wastewater: the unknown photo-deactivation process of low-lying excited states of isothiazolinones. A non-adiabatic dynamics investigation

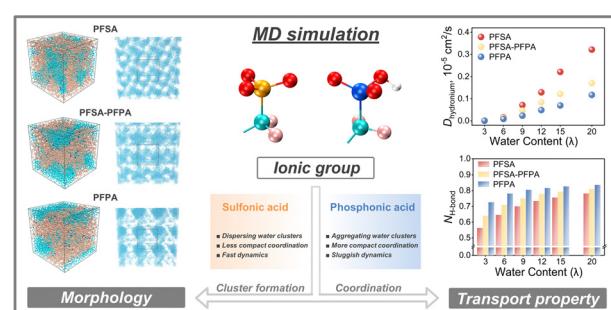
Bruno Bercini de Araújo and Paulo Fernando Bruno Gonçalves*



12806

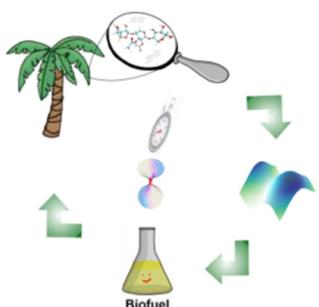
Effect of ionic groups on the morphology and transport properties in a novel perfluorinated ionomer containing sulfonic and phosphonic acid groups: a molecular dynamics study

Zongwei Zhang, Rui Cui, Xuesong Jiang, Chunyang Yu* and Yongfeng Zhou*



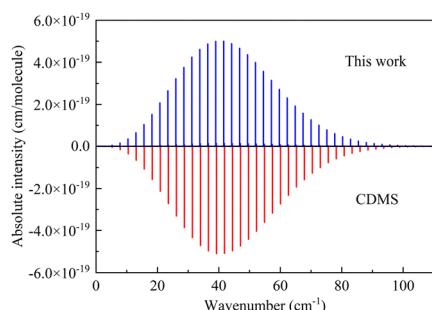
RESEARCH PAPERS

12820

**Hemicellulose pyrolysis: mechanism and kinetics of functionalized xylopyranose**

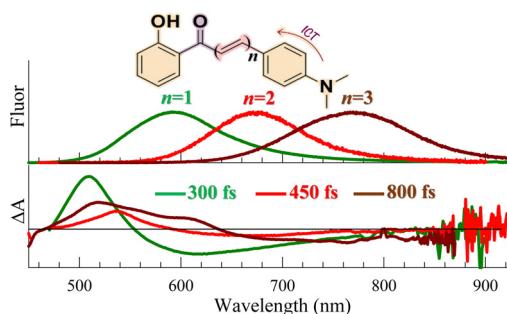
Leandro Ayarde-Henriquez,* Jacopo Lupi and Stephen Dooley*

12838

**High-temperature molecular line list of hydroboron monoxide (HBO)**

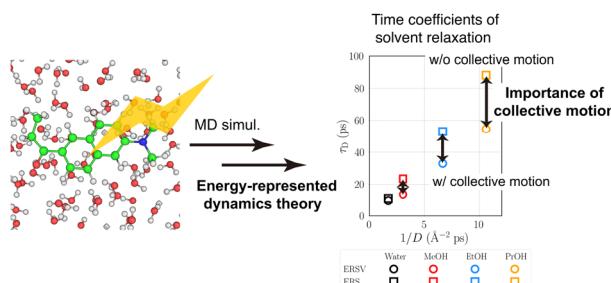
Ximing Li, Zhi Qin* and Linhua Liu*

12844

**Enhanced intramolecular charge transfer and near-infrared fluorescence in 4-dimethylamino-chalcone analogues through extended conjugation: synthesis, photophysical properties, and theoretical modelling**

Balqees S. Al-Saadi, A. Ramadan Ibrahim, John Husband,* Ahmed H. Ismail, Younis Baqi* and Osama K. Abou-Zied*

12852

**Solvation dynamics on the diffusion timescale elucidated using energy-represented dynamics theory**

Kazuya Okita, Natsuumi Ito, Nozomi Morishita-Watanabe, Hiroshi Umakoshi, Kento Kasahara* and Nobuyuki Matubayasi

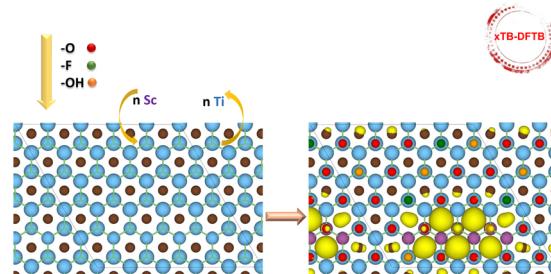
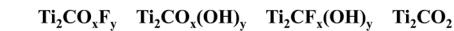


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Prediction of induced magnetism in 2D Ti_2C based MXenes by manipulating the mixed surface functionalization and metal substitution computed by xTB model Hamiltonian of the DFTB method

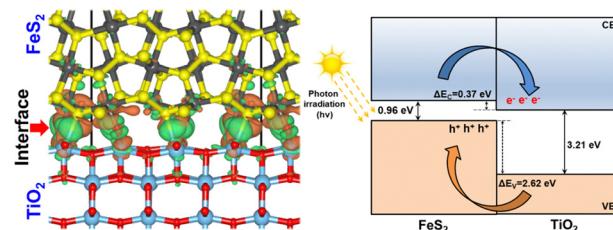
Taoufik Sakhraoui* and František Karlický



12869

Unraveling the origin of the high photocatalytic properties of earth-abundant $\text{TiO}_2/\text{FeS}_2$ heterojunctions: insights from first-principles density functional theory

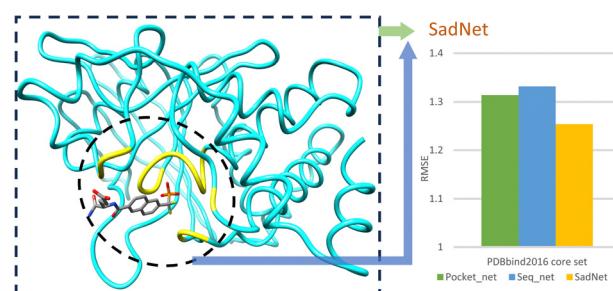
Oluwayomi F. Awe, Henry I. Eya, Ricardo Amaral, Nikhil Komalla, Pascal Nbelayim and Nelson Y. Dzade*



12880

SadNet: a novel multimodal fusion network for protein–ligand binding affinity prediction

Qiansen Hong, Guoqiang Zhou,* Yuke Qin, Jun Shen and Haoran Li



CORRECTIONS

12892

Correction: Quantifying the ion coordination strength in polymer electrolytes

Rassmus Andersson, Guiomar Hernández and Jonas Mindemark*



CORRECTIONS

12893

Correction: Quantum and semiclassical studies of nonadiabatic electronic transitions between N(⁴S) and N(²D) by collisions with N₂

Dandan Lu, Breno R. L. Galvão, Antonio J. C. Varandas and Hua Guo*

