

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(16) 12249–12896 (2024)



Cover

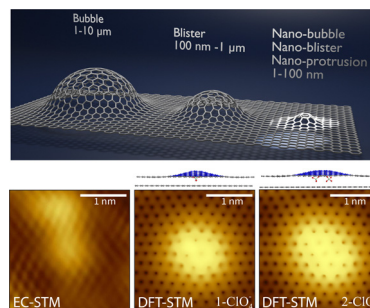
See Hussam Bouaamlat, Luca Tortora *et al.*, pp. 12269–12281. Image reproduced by permission of Luca Tortora from *Phys. Chem. Chem. Phys.*, 2024, 26, 12269. Image created via Blender Foundation (www.blender.org).

RESEARCH PAPERS

12269

Nano-protrusions in intercalated graphite: understanding the structural and electronic effects through DFT

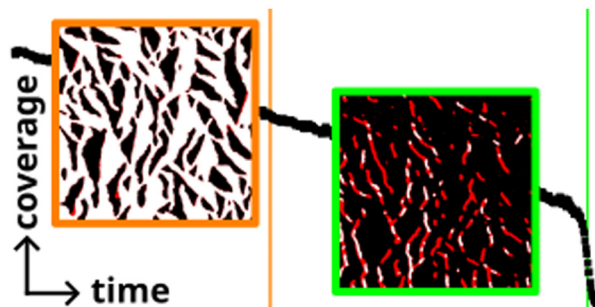
Hussam Bouaamlat,* Ari Paavo Seitsonen, Gianlorenzo Bussetti, Rossella Yivlialin, Stefania De Rosa, Paolo Branchini and Luca Tortora*



12282

Impact of long-range attraction on desorption kinetics

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



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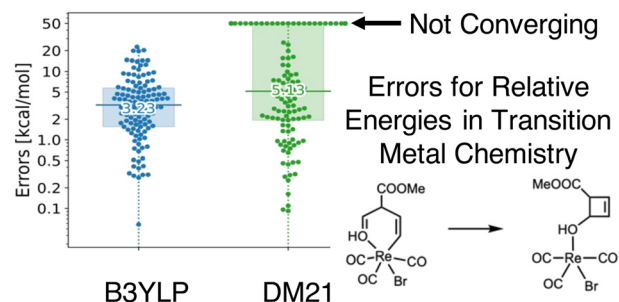
**Fundamental questions
Elemental answers**

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12289

Deep Mind 21 functional does not extrapolate to transition metal chemistry

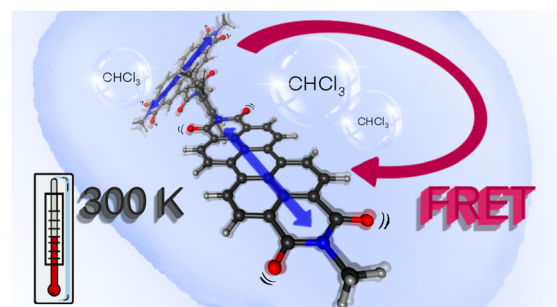
Heng Zhao, Tim Gould and Stefan Vuckovic*



12299

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

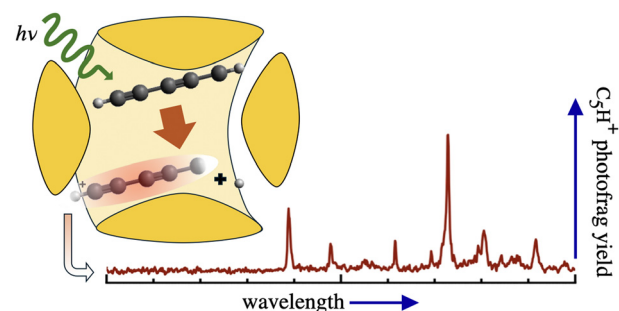
Richard Jacobi and Leticia González*



12306

Gas-phase electronic spectra of HC_{2n+1}H⁺ ($n = 2-6$) chains

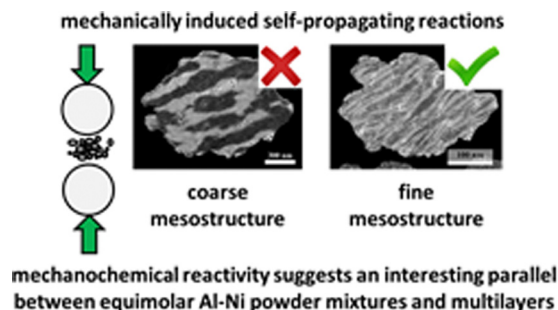
Samuel J. P. Marlton, Chang Liu, Patrick Watkins and Evan J. Bieske*



12316

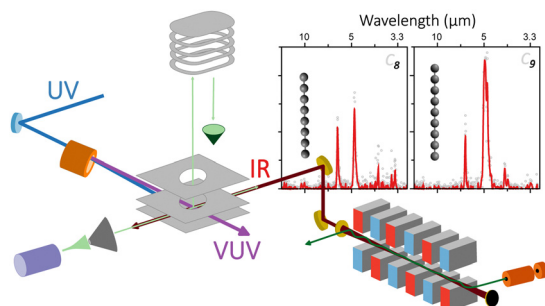
Mechanochemical ignition of self-propagating reactions in equimolar Al–Ni powder mixtures and multilayers

Maria Carta and Francesco Delogu*



RESEARCH PAPERS

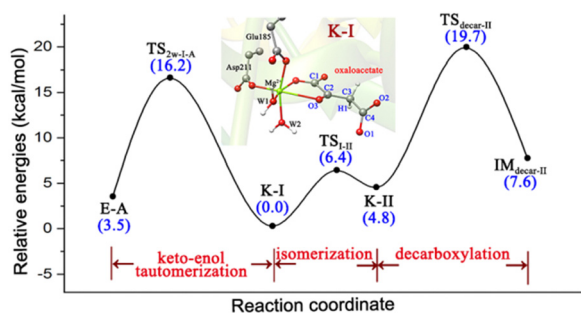
12324



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

Piero Ferrari,* Alexander K. Lemmens and Britta Redlich

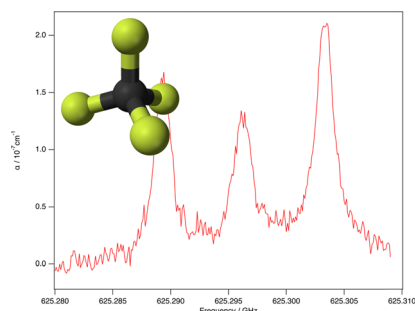
12331



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

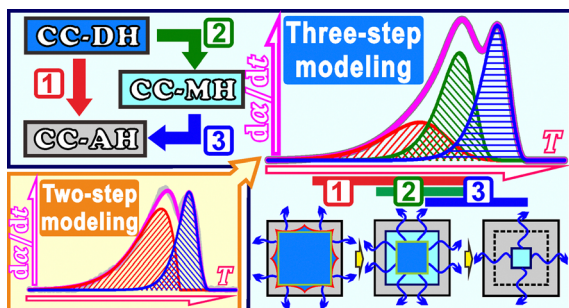
Xinyi Li, Fa-Guang Zhang, Jun-An Ma* and Yongjun Liu*

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Unrivalled accuracy in measuring rotational transitions of greenhouse gases: THz CRDS of CF₄

Fabien Simon, Arnaud Cuisset,* Coralie Elmaleh, Francis Hindle, Gaël Mouret, Michaël Rey, Cyril Richard and Vincent Boudon

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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*

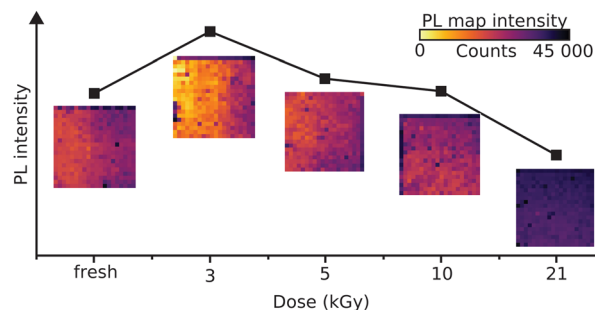


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Gamma-ray dose threshold for MAPbI₃ solar cells

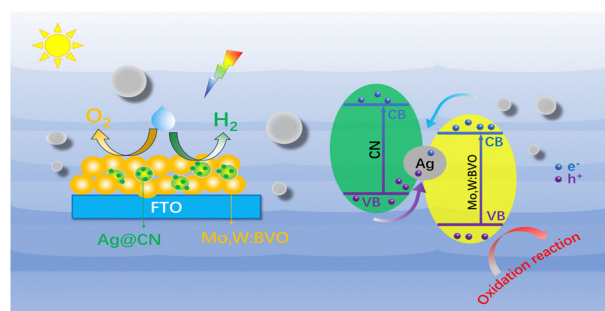
A. G. Boldyreva,* A. V. Novikov, V. G. Petrov,
A. N. Zhivchikova, M. M. Tepliakova and K. J. Stevenson



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

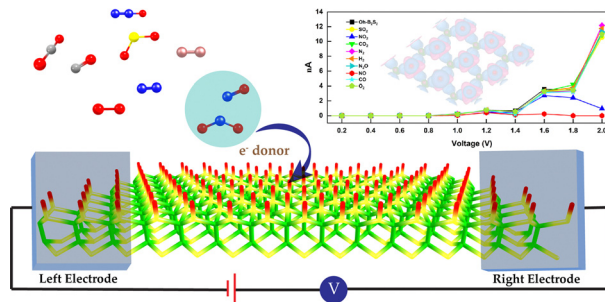
Shuai Chu, Wei Zhai, Lei Ding, Lin Wang, Jie Li and
Zhengbo Jiao*



12386

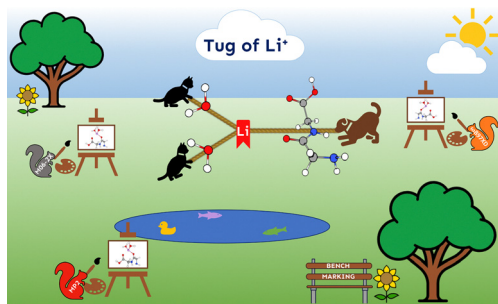
Realization of efficient and selective NO and NO₂ detection via surface functionalized h-B₂S₂ monolayer

Upasana Nath and Manabendra Sarma*



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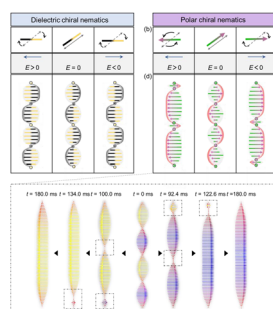
12406



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

Katharina A. E. Meyer and Etienne Garand*

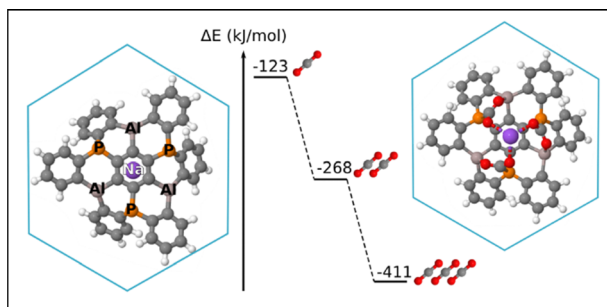
12422



Response of helielectric nematics under an in-plane electric field

Satoshi Aya,* Hao Xu, Huaqian Long, Muhan Yiliu, Yu Zou and Mingjun Huang

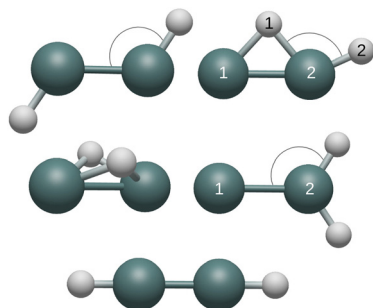
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A multi-FLP approach for CO_2 capture: investigating nitrogen, boron, phosphorus and aluminium doped nanographenes and the influence of a sodium cation

Maxime Ferrer, Ibon Alkorta,* José Elguero and Josep M. Oliva-Enrich

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A wealth of structures for the Ge_2H_2^+ radical cation: comparison of theory and experiment

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

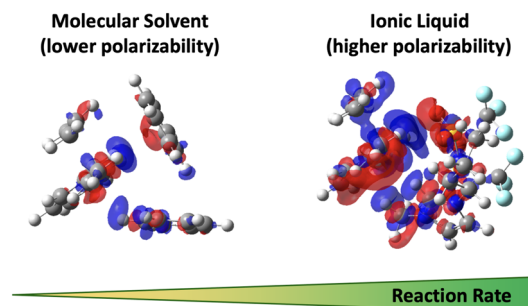


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Unravelling ionic liquid solvent effects for a non-polar Cope rearrangement reaction

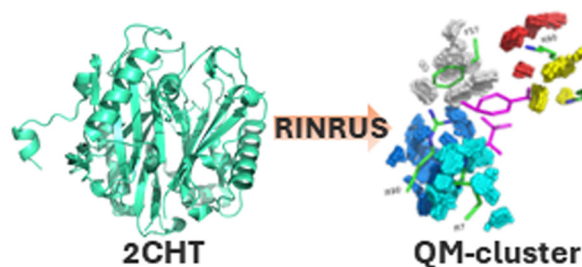
Gavin J. Smith, Spyridon Koutsoukos, Ben Lancaster, Julian Becker, Tom Welton and Patricia A. Hunt*



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

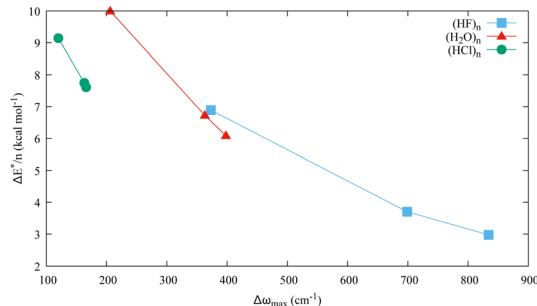
Donatus A. Agbaglo, Thomas J. Summers, Qianyi Cheng and Nathan J. DeYonker*



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Systematic analysis of electronic barrier heights and widths for concerted proton transfer in cyclic hydrogen bonded clusters: $(\text{HF})_n$, $(\text{HCl})_n$ and $(\text{H}_2\text{O})_n$ where $n = 3, 4, 5$

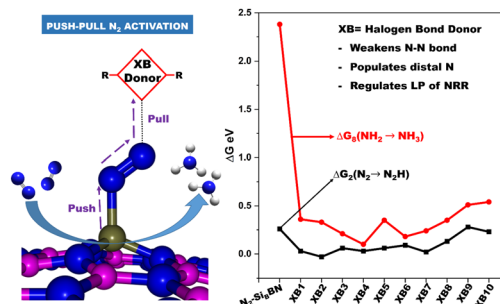
Yuan Xue, Thomas More Sexton, Johnny Yang and Gregory S. Tschumper*



12495

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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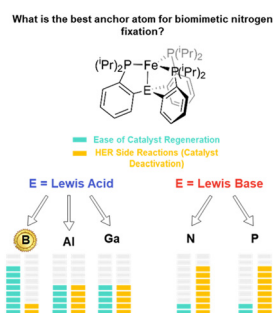
12510



Bridging the gap: viable reaction pathways from tetrahydrene to benzyne

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

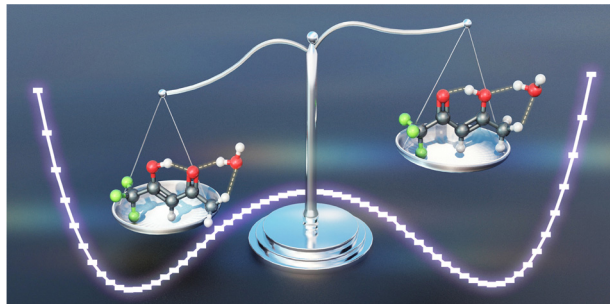
12520



Role of Lewis acid/base anchor atoms in catalyst regeneration: a comprehensive study on biomimetic EP₃Fe nitrogenases

Joseph Kfoury and Julianna Oláh*

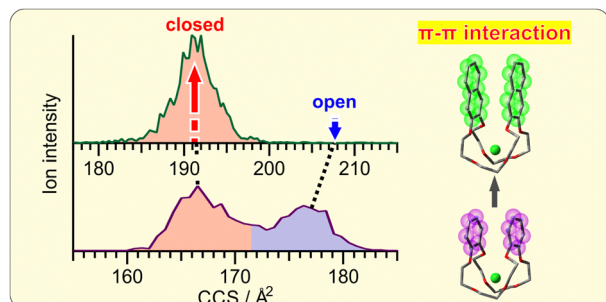
12530



A rotational spectroscopy study of microsolvation effects on intramolecular proton transfer in trifluoroacetylacetone-(H₂O)₁₋₃

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

12537



Intra-host π-π interactions in crown ether complexes revealed by cryogenic ion mobility-mass spectrometry

Ryosuke Ito, Keiji Ohshimo* and Fuminori Misaizu*

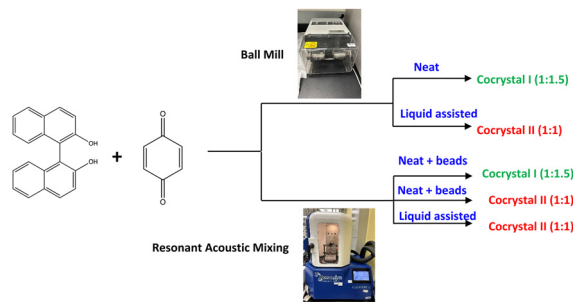


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Comparison of mechanochemical methods in the synthesis of binaphthol–benzoquinone based cocrystals

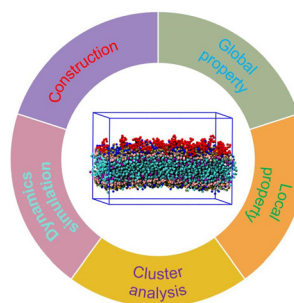
Siddarth Nagapudi and Karthik Nagapudi*



12552

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

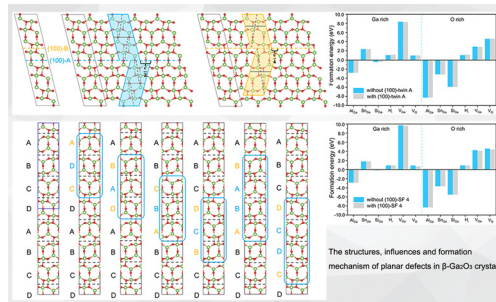
Yongkang Lyu, Shuo Chen, Yu Zhao, Hongxiu Yuan, Chenyang Zhang, Changzhe Zhang and Qingtian Meng*



12564

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

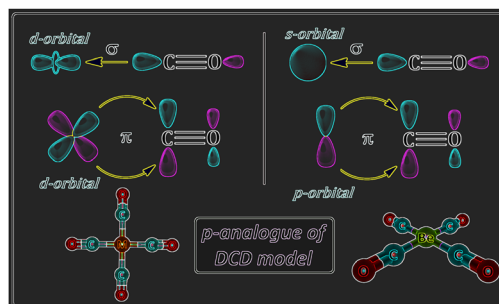
Qi Li, Xin Guan, Yu Zhong, Zhitai Jia,* Yang Li* and Na Lin*



12573

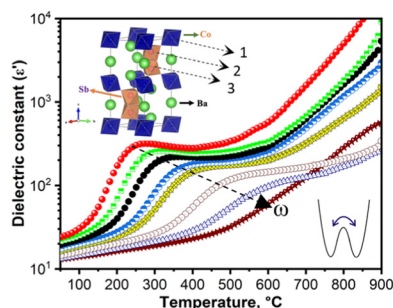
Beryllium carbonyl Be(CO)_n (n = 1–4) complex: a p-orbital analogy of Dewar–Chatt–Duncanson model

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



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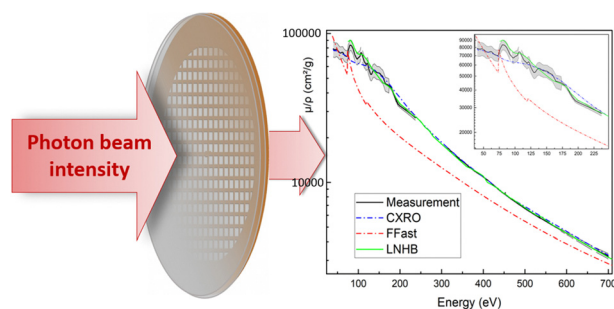
12580



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

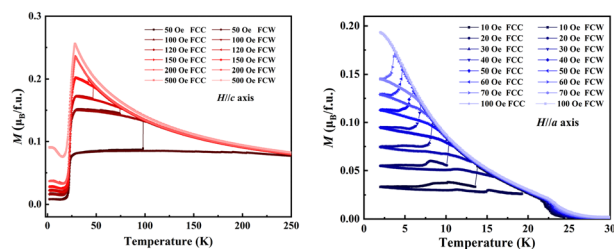
12587



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

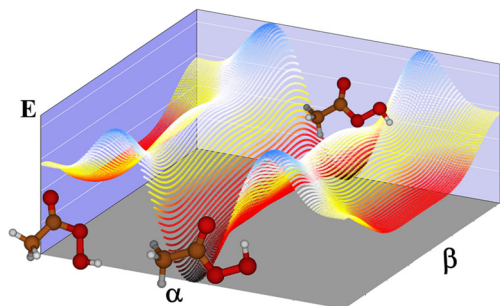
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Low field controllable continuous spin switching in the thulium–ytterbium single crystal

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

12600



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 Najjar and Maria Luisa Senent*



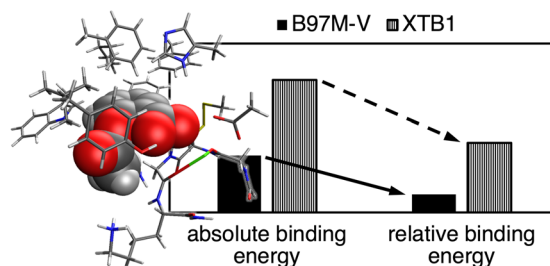
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12610

Sorting drug conformers in enzyme active sites: the XTB way

Bun Chan,* William Dawson and Takahito Nakajima

Molecule–Environment Interaction

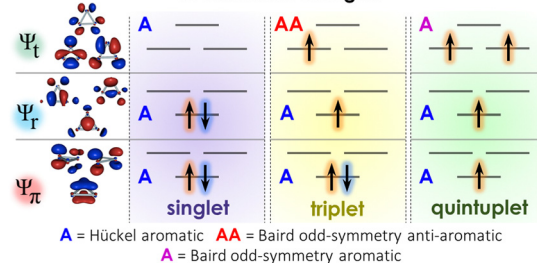


12619

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*

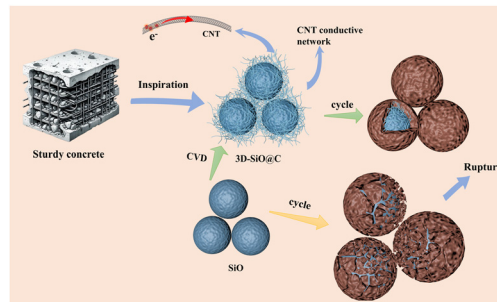
Mandado's 2n+1 Rule: Spin Separated Aromaticity in Triel Metal Triangles



12628

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

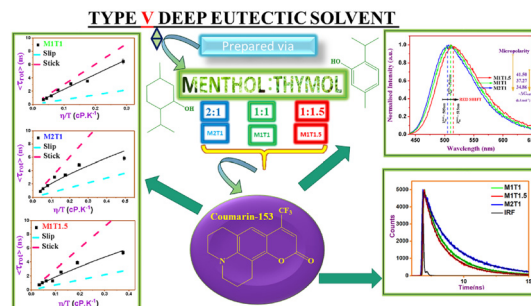
Xiaobo Duan,* Jiaao Yu, Yancai Liu, Yanqiang Lan, Jian Zhou, Birou Lu, Lina Zan, Zimin Fan and Lei Zhang*



12638

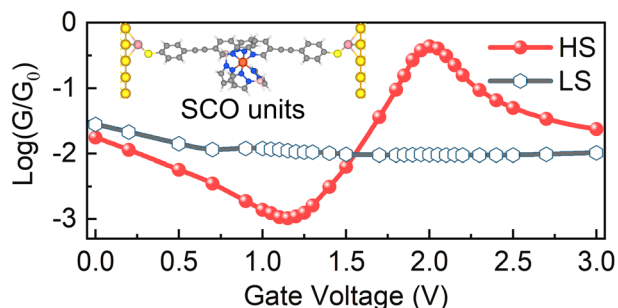
Solute dynamics of a hydrophobic molecule in a menthol–thymol based type-V deep eutectic solvent: effect of composition of the components

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



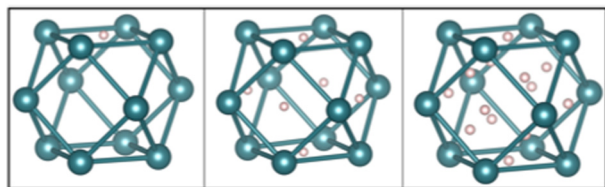
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**Fano resonance in molecular junctions of spin crossover complexes**

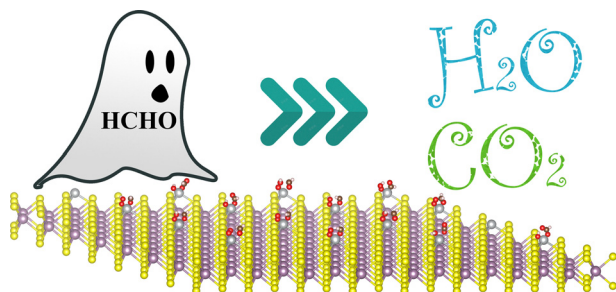
Hua Hao,* Honghao Li, Ting Jia, Yanhong Zhou and Xiaohong Zheng*

12661

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

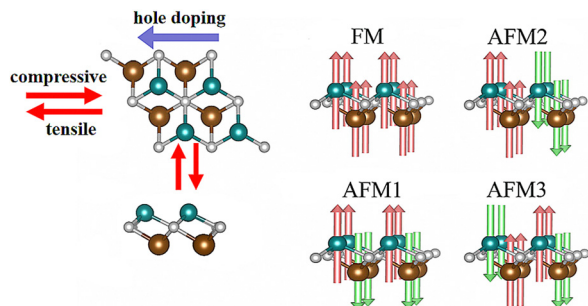
Alexander Muñoz,* Ivana Matanovic, Brendan Gifford, Sven Rudin, Troy Holland and Travis Jones*

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**A first-principles study on Ni-decorated MoS_2 for efficient formaldehyde degradation over a wide temperature range**

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

12681

**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*

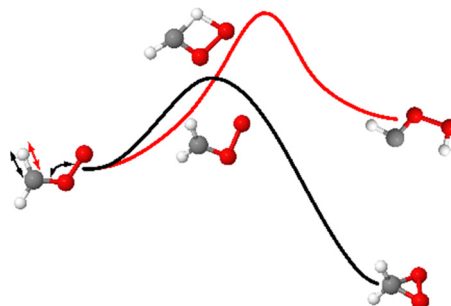


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OH-Formation following vibrationally induced reaction dynamics of H_2COO

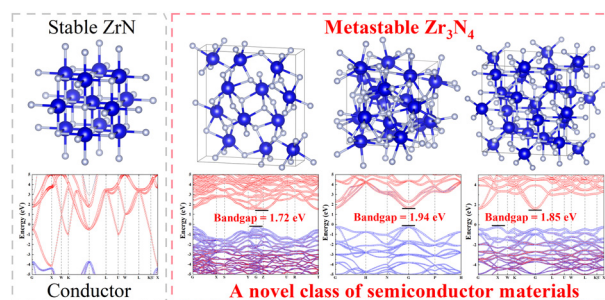
Kaisheng Song, Meenu Upadhyay and Markus Meuwly*



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Electronic and elastic properties of metastable Zr_3N_4 : a joint experimental and theoretical study

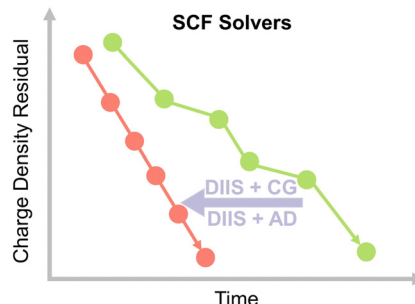
Yuhe Liu, Kunlun Wang, Nina Ge, Hui Sun, Bo Dai and Yong Wang*



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

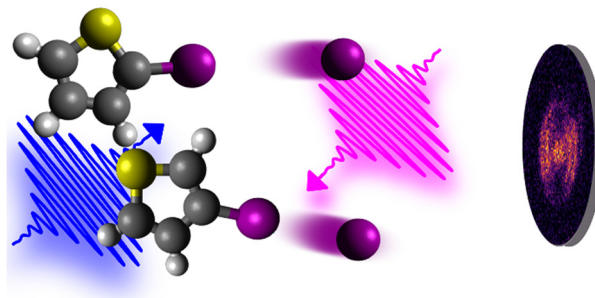
Zhaosheng Zhang,* Sijia Liu and Yingjie Zhang



12725

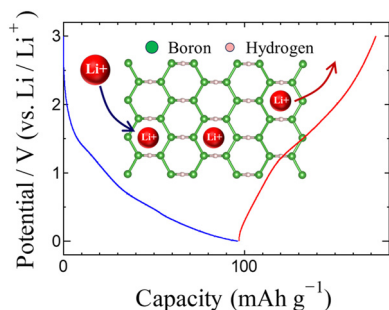
Exploring the ultrafast and isomer-dependent photodissociation of iodothiophenes via site-selective ionization

W. O. Razmus, F. Allum, J. Harries, Y. Kumagai, K. Nagaya, S. Bhattacharyya, M. Britton, M. Brouard, P. H. Bucksbaum, K. Cheung, S. W. Crane, M. Fushitani, I. Gabalski, T. Gejo, A. Ghrist, D. Heathcote, Y. Hikosaka, A. Hishikawa, P. Hockett, E. Jones, E. Kukk, H. Iwayama, H. V. S. Lam, J. W. McManus, D. Milesevic, J. Mikosch, S. Minemoto, A. Niozu, A. J. Orr-Ewing, S. Owada, D. Rolles, A. Rudenko, D. Townsend, K. Ueda, J. Unwin, C. Vallance, A. Venkatachalam, S.-i. Wada, T. Walmsley, E. M. Warne, J. L. Woodhouse, M. Burt, M. N. R. Ashfold, R. S. Minns* and R. Forbes*



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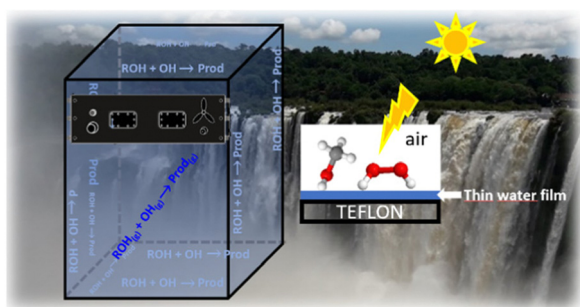
12738



Lithium-ion battery electrode properties of hydrogen boride

Tatsuya Akiyama, Marina Ukai, Yosuke Ishii,*
Shinji Kawasaki and Yoshiyuki Hattori

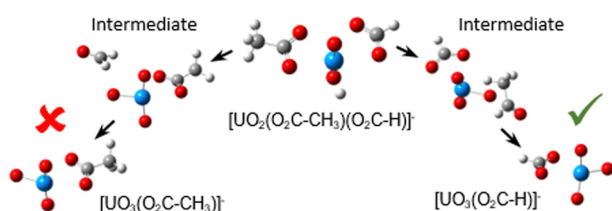
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Understanding the active role of water in laboratory chamber studies of reactions of the OH radical with alcohols of atmospheric relevance

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

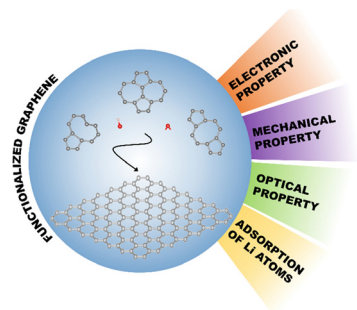
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Reactions of gas-phase uranyl formate/acetate anions: reduction of carboxylate ligands to aldehydes by intra-complex hydride attack

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

12764



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*

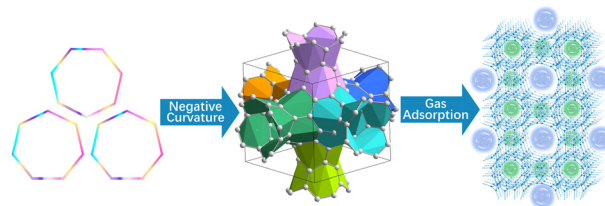


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The smallest Schwarzite carbon with only heptagonal carbon rings

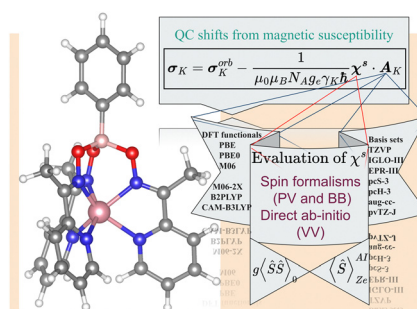
Meng Hu, Junwen Huang, Lu Shi, Jing Hua,*
Lingyu Liu, Julong He and Jianning Ding



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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

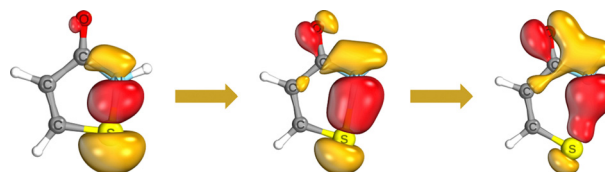
Md. Ashraful Islam* and Andrew J. Pell*



12799

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

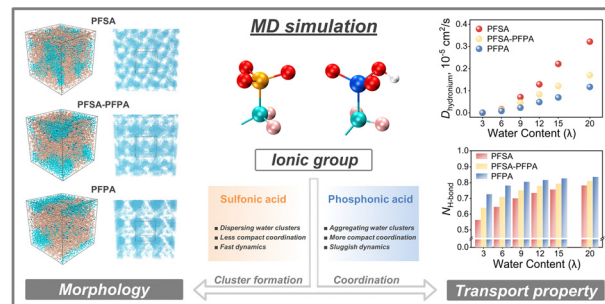
Bruno Bercini de Araújo and Paulo Fernando Bruno Gonçalves*



12806

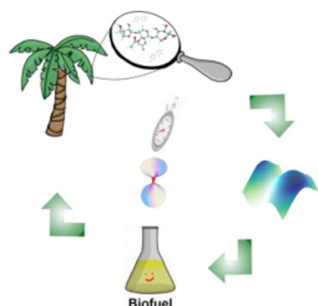
Effect of ionic groups on the morphology and transport properties in a novel perfluorinated ionomer containing sulfonic and phosphonic acid groups: a molecular dynamics study

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



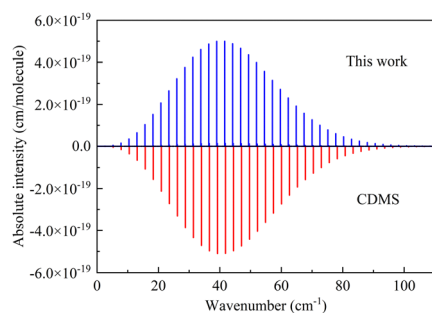
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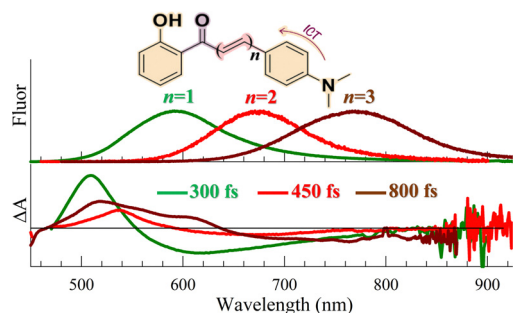
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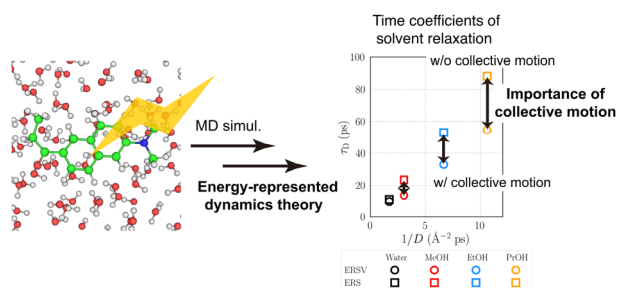
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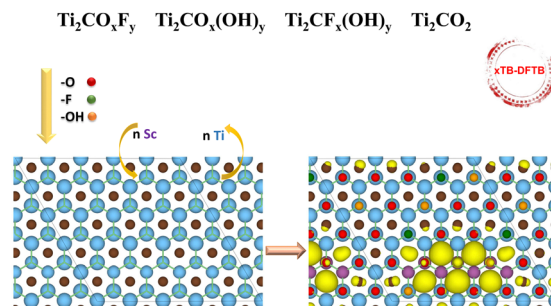


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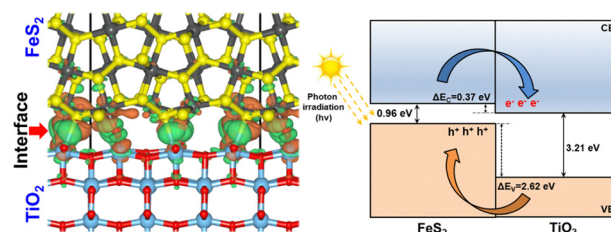
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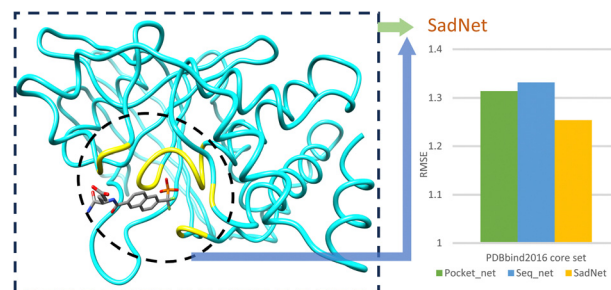
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CORRECTIONS

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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 N_2

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

