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Cover

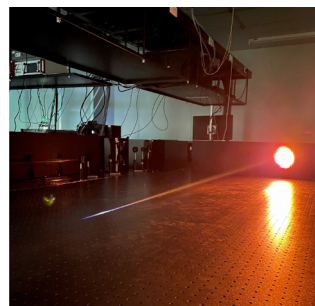
See Thomas Golin Almeida, Sommer L. Johansen *et al.*, pp. 23570–23587. Image reproduced by permission of Thomas Golin Almeida from *Phys. Chem. Chem. Phys.*, 2024, 26, 23570.

REVIEWS

23528

Fluorescence and lasing of neutral nitrogen molecules inside femtosecond laser filaments in air: mechanism and applications

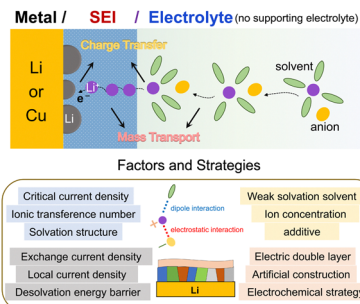
Haicheng Mei, Hongbing Jiang, Aurélien Houard, Vladimir Tikhonchuk, Eduardo Oliva, André Mysyrowicz, Qihuang Gong, Chengyin Wu and Yi Liu*



23544

Kinetic understanding of lithium metal electrodeposition for lithium anodes

Rong Fang, Yu-Xi Li, Wei-Wei Wang, Yu Gu* and Bing-Wei Mao*



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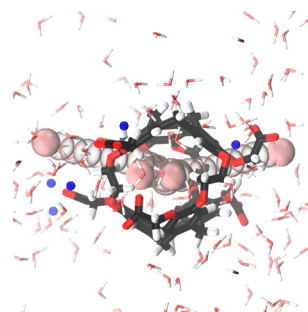
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COMMUNICATIONS

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Acceleration of xenon kick-out exchange in a cryptophane host explained by *ab initio* simulation

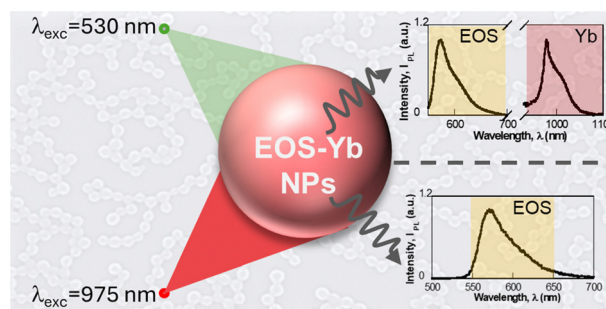
Rodolphe Pollet,* Jean-Pierre Dognon and Patrick Berthault



23566

NIR-triggered upconversion and sensitized NIR-emission in Yb-based Eosin Y lake doped latex nanoparticles

Rita B. Cevallos-Toledo, Delia Bellezza, María González-Béjar* and Julia Pérez-Prieto*

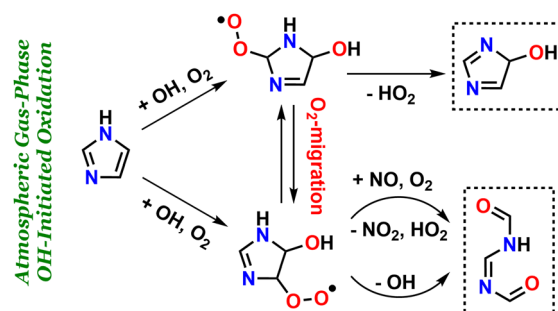


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23570

Theoretical analysis of the OH-initiated atmospheric oxidation reactions of imidazole

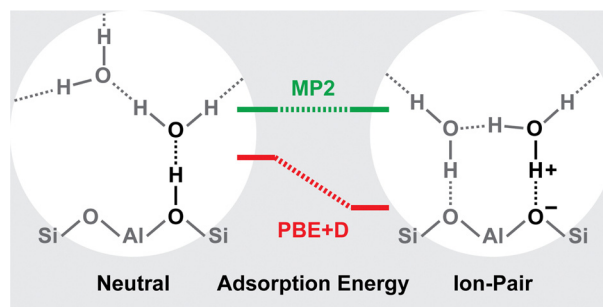
Thomas Golin Almeida,* Carles Martí, Theo Kurtén, Judit Zádor and Sommer L. Johansen*



23588

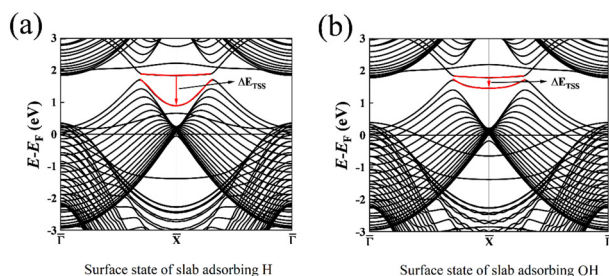
Chemically accurate predictions for water adsorption on Brønsted sites of zeolite H-MFI

Henning Windeck, Fabian Berger and Joachim Sauer*



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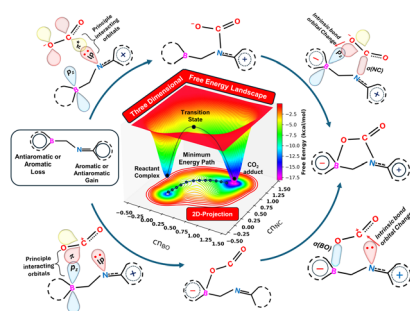
23600



Variation of topological surface states of nodal line semimetal MgB_2 resulting from adsorption of hydrogen, hydroxide, and water molecules

Pangdong Zhu, Kun Bu,* Ruzhi Wang and Changhao Wang*

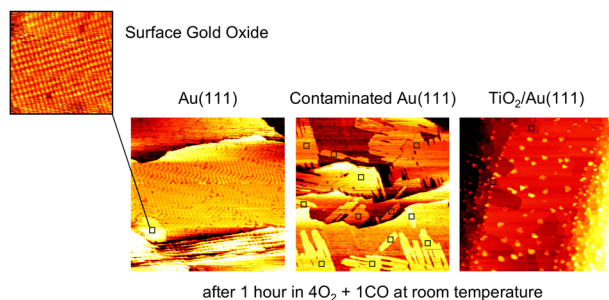
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Orbital and free energy landscape expedition towards the unexplored catalytic realm of aromatically modified FLPs for CO_2 sequestration

Mohammad Faizan, Madhumita Chakraborty, Dinesh Bana and Ravinder Pawar*

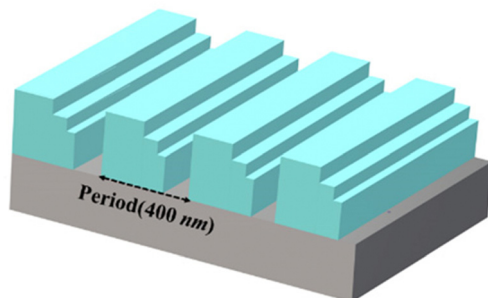
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Gold oxide formation on $\text{Au}(111)$ under CO oxidation conditions at room temperature

Sabine Wenzel,* Dajo Boden and Irene M. N. Groot

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Broadband and weak-dispersion nonlinear response enhancement in the epsilon-near-zero region of a nano-stepped metasurface

Yanxin Lu, Jiahui Zheng, Feilian Zhang, Qiqi Guo, Yunfei Song, Jiannan Dong and Yihang Chen*

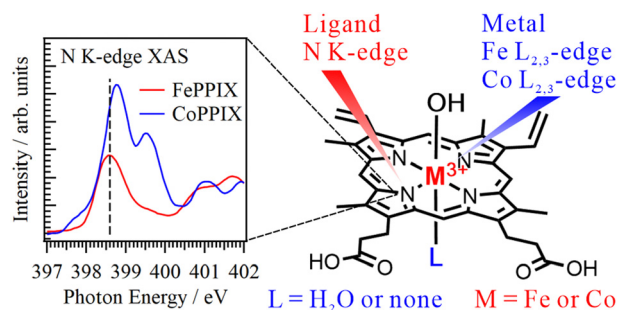


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Metal–ligand delocalization of iron and cobalt porphyrin complexes in aqueous solutions probed by soft X-ray absorption spectroscopy

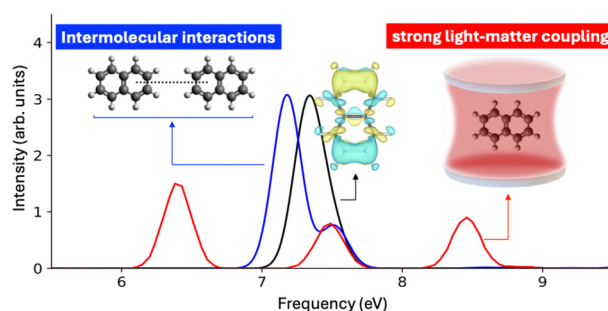
Masanari Nagasaka,* Shota Tsuru and Yasuyuki Yamada



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Modulating molecular plasmons in naphthalene via intermolecular interactions and strong light–matter coupling

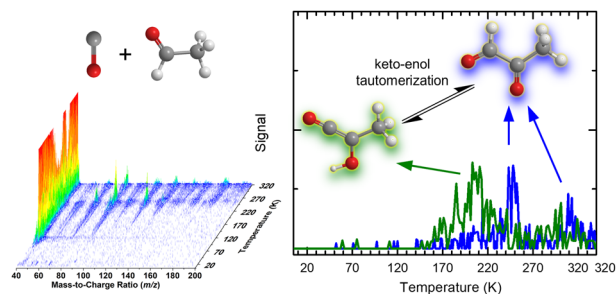
Zhen Liu* and Xiao Wang*



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Formation of methylglyoxal ($\text{CH}_3\text{C}(\text{O})\text{CHO}$) in interstellar analog ices – a key intermediate in cellular metabolism

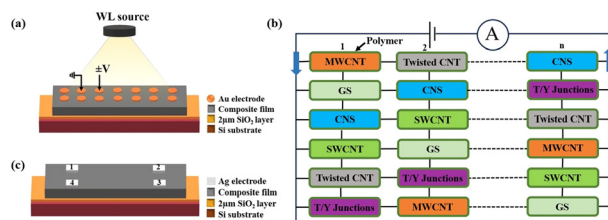
Jia Wang, Joshua H. Marks, Evgenia A. Batrakova, Sergey O. Tuchin, Ivan O. Antonov* and Ralf I. Kaiser*

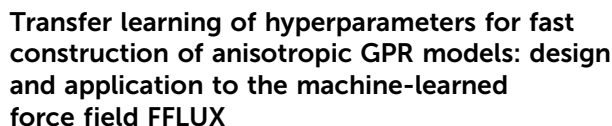


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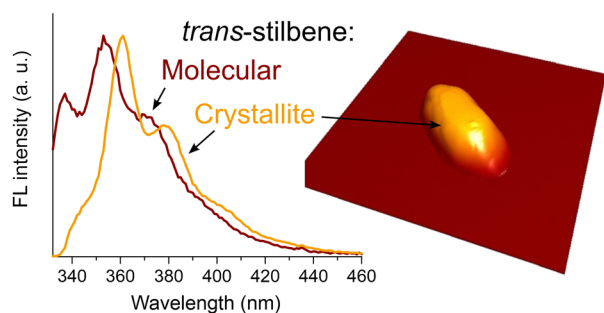
Electrical nature of randomly oriented low-dimensional structural hybrids of carbon

Sonia Saini, Kuntala Bhattacharjee* and Girish M. Gouda



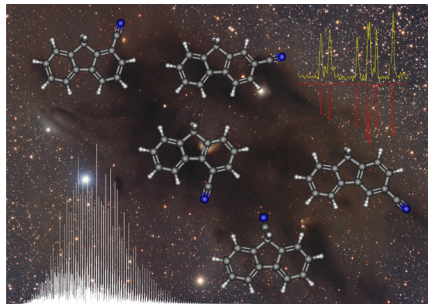


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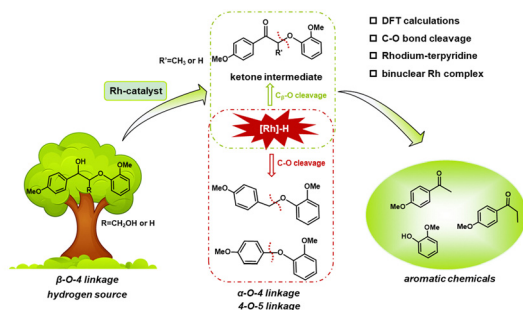
***trans*-Stilbene aggregates and crystallites in polystyrene films: microscopy and spectroscopy studies**

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Marija Jankunec, Jevgenij Chmeliov,
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Rotational spectra of five cyano derivatives of fluorene

Carlos Cabezas,* Jesús Janeiro, Amanda L. Steber,
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Redox-neutral depolymerization of lignin-derived aryl ethers catalyzed by Rh(III)-complexes: a mechanistic insight

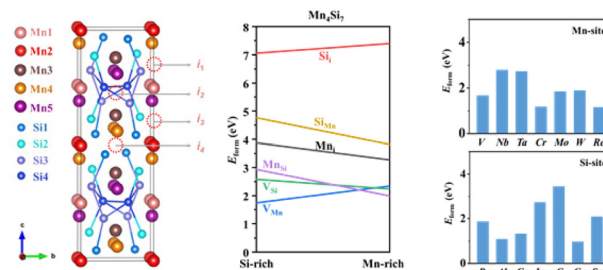
Yan Zhang, Yafei Luo, Changwei Hu, Dianyong Tang*
and Zhishan Su*

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A first-principles study of the electronic structure and point defects in higher manganese silicide Mn_4Si_7

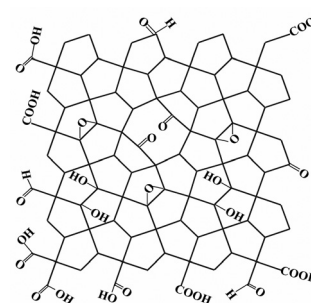
Jun Chai,* Guangshu Li, Mingping He and Hangjia Shen



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Regulation of $\text{C}=\text{C}$ bonds in penta-graphene by oxidative functionalization: a prototype of penta-graphene oxide (PGO)

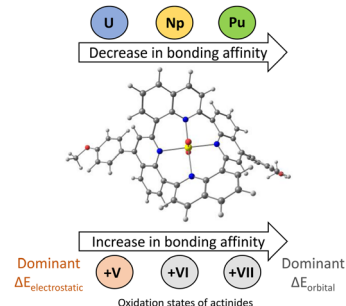
Kaixuan Jin and Xiaojie Liu*



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High-valent actinyl (AnO_2 ; $\text{An} = \text{U}, \text{Np}$ and Pu) complexation with TETraQuinoline (TEQ) ligand – a DFT study

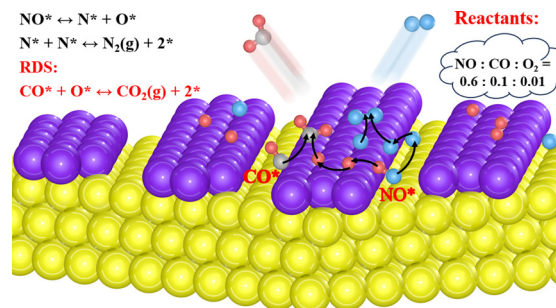
Abigail Jennifer G and Elumalai Varathan*



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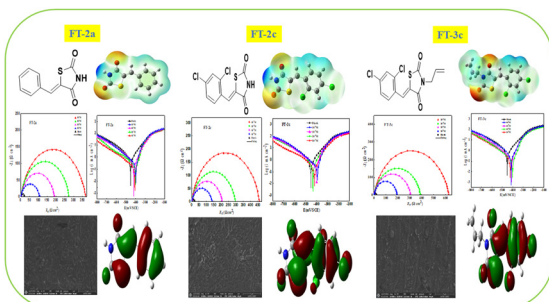
Design and screening of bimetallic catalysts for nitric oxide reduction by CO: a study of kinetic Monte Carlo simulation based on first-principles calculations

Caimu Wang, Renyi Li and Wei Guo*



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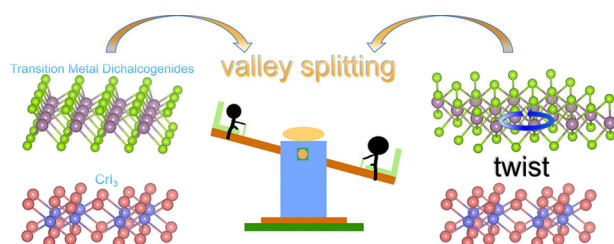
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Experimental and theoretical approach for a better understanding of the mechanisms of adsorption and inhibition of corrosion for carbon steel by thiazolidine derivatives in 1 M HCl medium

L. Chahir, N. Benzbiria, F. Z. Tahri, M. El Faydy, F. Benhiba, D. Benmessaoud Left, M. Zertoubi, I. Warad, M. Allali, K. Bougrin and A. Zarrouk*

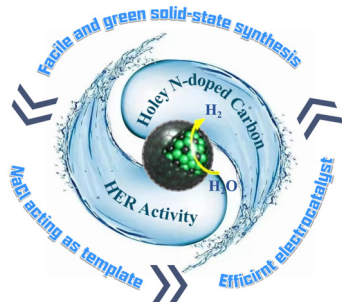
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First-principles study of valley splitting of transition-metal dichalcogenides in MX_2/CrI_3 ($M = W, Mo$; $X = S, Se, Te$) van der Waals heterostructures

Mei Ge, Leiting Chu, Fanmin Zeng, Zhongyin Cao* and Junfeng Zhang*

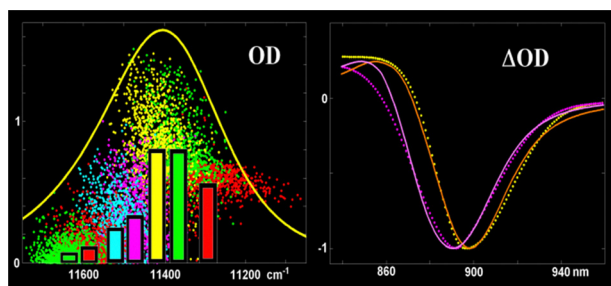
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Cooperation between holey N-doped carbon and Ni nanoparticles as an efficient electrocatalyst for the hydrogen evolution reaction

Wenchong Zhang, Heng Ke, Mixue Gong, Jie Yang, Ningbo Yu, Yanan Xue, Jianzhi Wang* and Faquan Yu*

23800



Multiexciton spectra of molecular aggregates: application to photosynthetic antenna complexes

Vladimir I. Novoderezhkin* and Andrei P. Razjivin

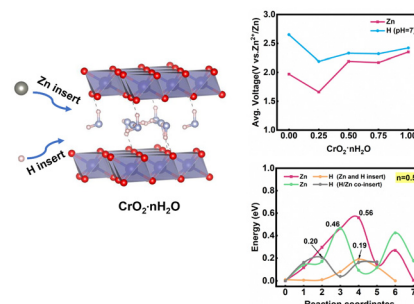


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Layered $\text{CrO}_2 \cdot n\text{H}_2\text{O}$ as a cathode material for aqueous zinc-ion batteries: *ab initio* study

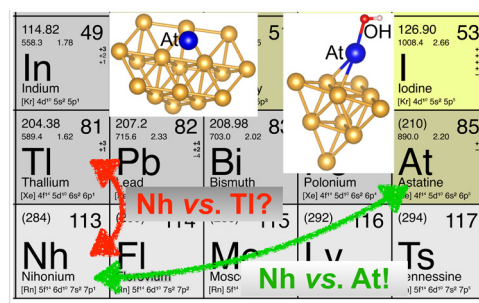
Lu Liu, Zixi He, Binghan Wu, Hongjia Song,*
Xiangli Zhong, Jinbin Wang, Daifeng Zou and
Juanjuan Cheng*



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Uncovering chemical homology of superheavy elements: a close look at astatine

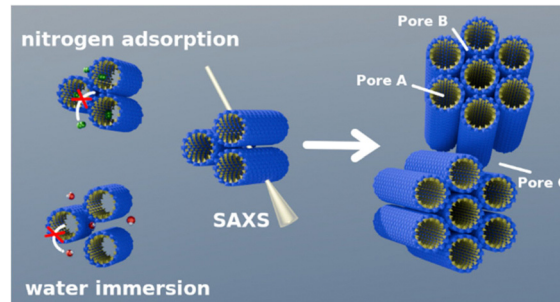
Yuriy A. Demidov, Alexander A. Shalaevsky,
Alexander V. Oleynichenko and Alexander A. Rusakov*



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Dried hybrid imogolite nanotubes as solids with a changeable surface area: an insight into textural properties based on the correlation between nitrogen gas adsorption, immersion calorimetry into water, and small angle X-ray scattering

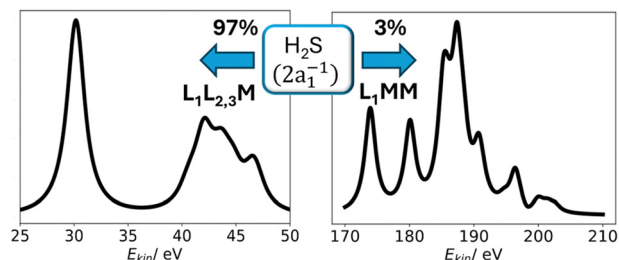
Ali Dhaini, Amine Geneste, Fadwa Alfadel Raad,
Pierre Picot, Gaëlle Martin-Gassin, Benedicte Prelot,
Pierre-Marie Gassin, Philippe Trens, Antoine Thill* and
Jerzy Zajac*



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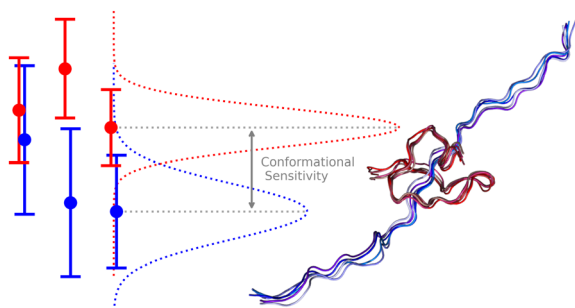
Ab initio treatment of molecular Coster–Kronig decay using complex-scaled equation-of-motion coupled-cluster theory

Jan Philipp Drennhaus, Anthuan Ferino-Pérez,
Florian Matz and Thomas-C. Jagau*



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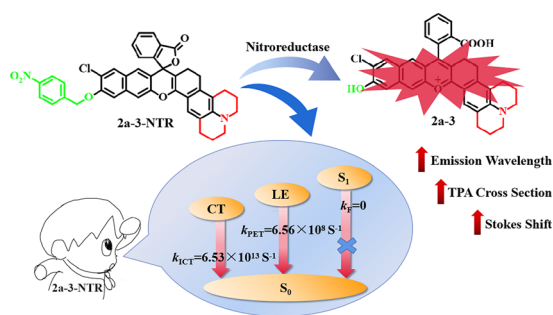
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Conformational dependence of chemical shifts in the proline rich region of TAU protein

Johannes Stöckelmaier and Chris Oostenbrink*

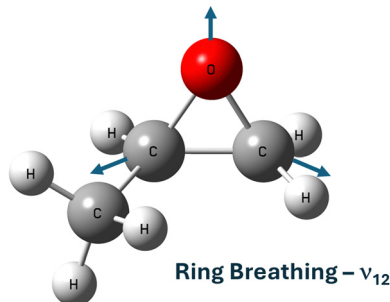
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Rational design of anthocyanidins-directed near-infrared two-photon fluorescent probes

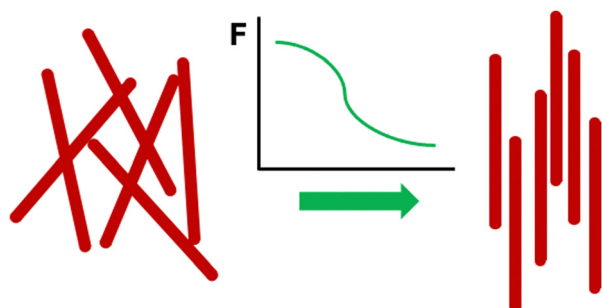
Xiu-e Zhang, Xue Wei, Wei-Bo Cui, Jin-Pu Bai, Aynur Matyusup, Jing-Fu Guo,* Hui Li and Ai-Min Ren*

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High-resolution infrared spectra and rovibrational analysis of the ν_{12} band of propylene oxide

Karel Vávra, Eileen Döring, Jan Jakob, Fabian Peterß, Martin Kaufmann, Pascal Stahl, Thomas F. Giesen* and Guido W. Fuchs

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Conditions under which a natural iterative method for calculating the orientation distribution of rodlike particles decreases the free energy at each step

Alan E. Berger

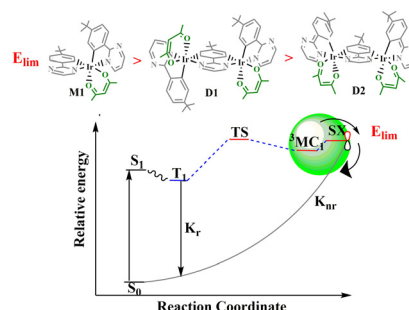


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The nonradiative decay mechanism of dinuclear iridium complexes: a density functional theory study

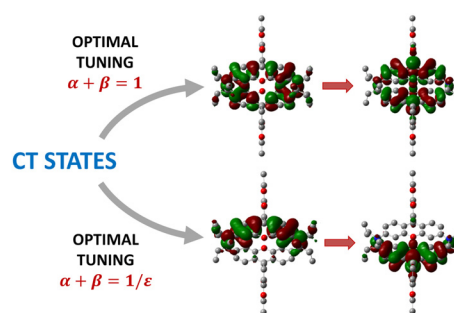
Guo-Jun Kang, Yong-Fei Wu, Xue-Feng Ren,*
Jie-Qiong Mei, Shi-Jian Lu and Xi Zeng*



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Optimal-tuning of range-separated density functionals to describe the optical and photophysical properties of rhodamine B dimers

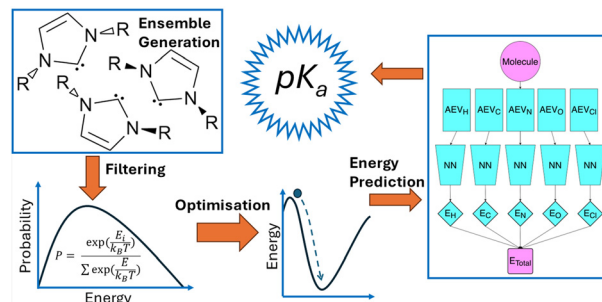
Giacomo Fanciullo, Carlo Adamo, Ivan Rivalta* and
Ilaria Ciofini*



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ANI neural network potentials for small molecule pK_a prediction

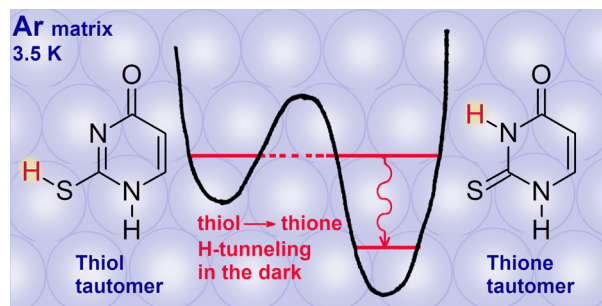
Ross James Urquhart, Alexander van Teijlingen and
Tell Tuttle*



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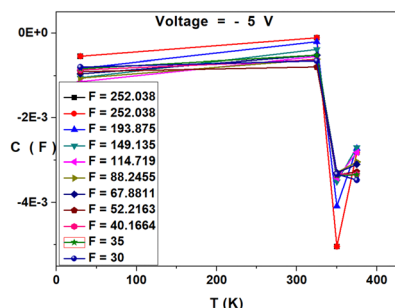
Intramolecular hydrogen-atom tunneling in matrix-isolated heterocyclic compounds: 2-thiouracil and its analogues

Hanna Rostkowska, Leszek Lapinski* and Maciej J. Nowak*



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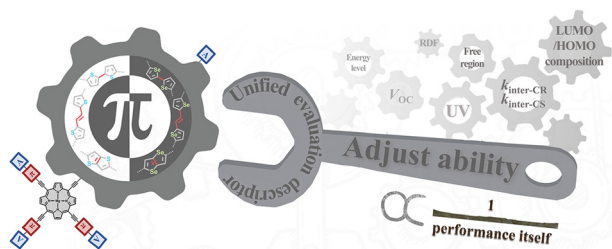
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Negative capacitance in Au/CuInGaSe₂/SiO₂/n-Si/Al Schottky barrier diode devices

A. Ashery, A. E. H. Gaballah and Mohamed A. Basyooni-M. Kabatas*

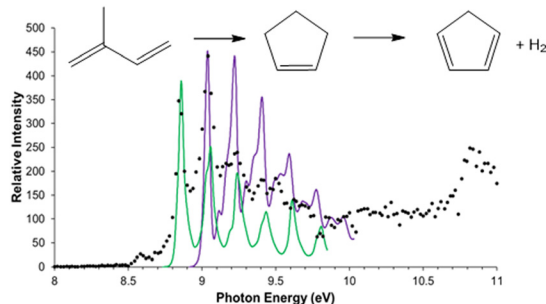
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A unified evaluation descriptor for π -bridges applied to metalloporphyrin derivatives

Meng-Tian Han, Liu Wu, Jian-Ping Wang, Ming-Yue Sui* and Guang-Yan Sun*

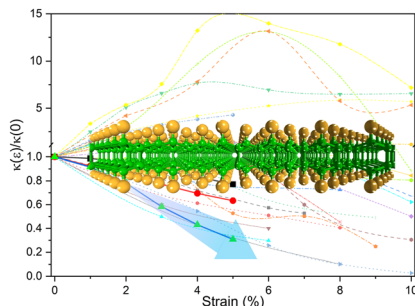
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Cyclopentene and cyclopentadiene formation in isoprene pyrolysis

Edgar White Buenger, Andras Bodi, Maxi A. Burgos-Paci and Paul M Mayer*

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Unveiling the strain-sensitive thermal transport properties of chlorinated diamane

Tingting Zhang* and Liyan Zhu*

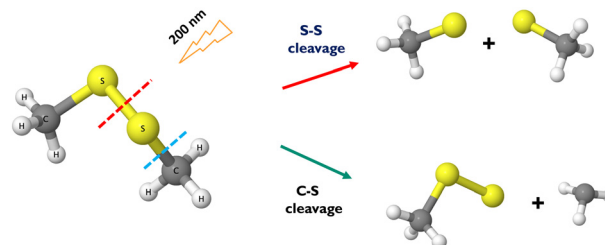


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Excited state electronic structure of dimethyl disulfide involved in photodissociation at ~ 200 nm

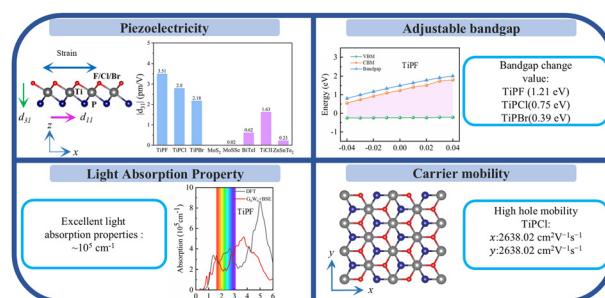
Varun Rishi, Neil C. Cole-Filipiak, Krupa Ramasesha* and Laura M. McCaslin*



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Theoretical study of piezoelectric and light absorption properties, and carrier mobilities of Janus TiPX (X = F, Cl, and Br) monolayers

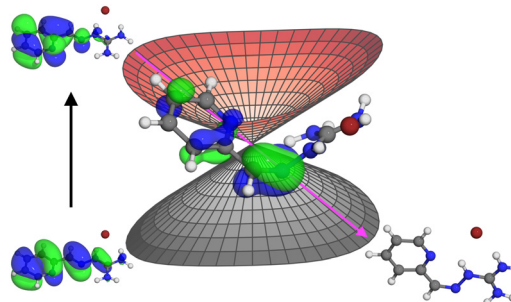
Tong-Tong Yan, Guo-Xiang Zhou,* Xiao-Long Jiang, Xu-Chen Qin and Jia Li



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Photoisomerization mechanism of iminoguanidinium receptors from spectroscopic methods and quantum chemical calculations

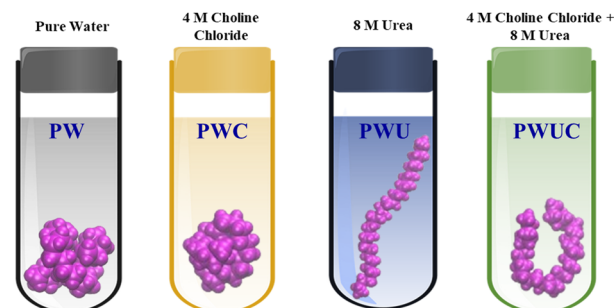
Duy-Khoi Dang, Jeffrey D. Einkauf, Xinyou Ma, Radu Custelcean, Ying-Zhong Ma,* Paul M. Zimmerman* and Vyacheslav S. Bryantsev*



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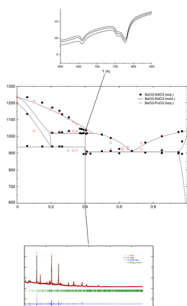
Osmolyte-induced conformational stabilization of a hydrophobic polymer

Pooja Nanavare, Soham Sarkar, Abhijit Bijay Jena and Rajarshi Chakrabarti*



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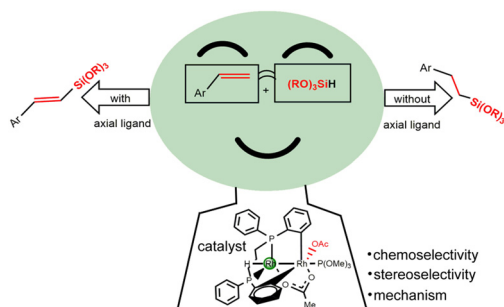
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Experimental investigation and thermodynamic modelling assessment of the $\text{AECl}_2\text{--NdCl}_3$ (AE = Sr, Ba) systems

D. C. Alders, D. J. Cette, R. J. M. Konings and A. L. Smith*

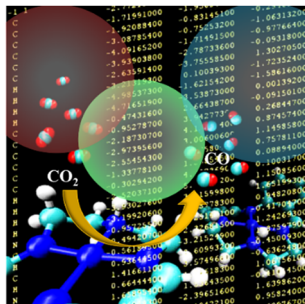
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Dirhodium(II) complex catalyzed dehydrosilylation of styrenes: theoretical investigations on the mechanism, selectivity, and ligand effects

Ziying Zhong, Qingzhong Li and Xiaoyan Li*

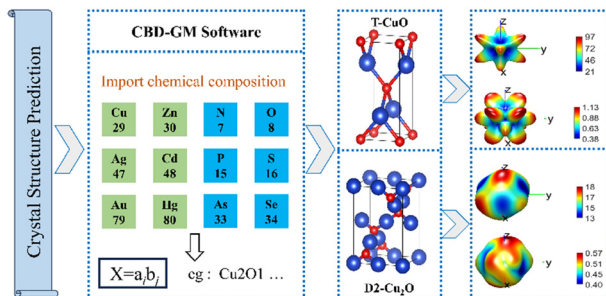
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Theoretical study of electrochemical reduction of CO_2 to CO using a nickel- N_4 -Schiff base complex

Wilasinee Santiwarodom, Pavee Apilardmongkol, Thanawit Kuamit and Vudhichai Parasuk*

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Crystal structure prediction and property calculation of copper–oxygen compounds using innovative search software from first principles

Jinrong Huo, Kai Zhang, Pengfei Liu, Haocong Wei and Chaozheng He*

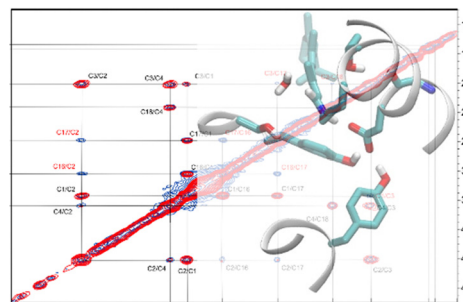


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The retinal chromophore environment in an inward light-driven proton pump studied by solid-state NMR and hydrogen-bond network analysis

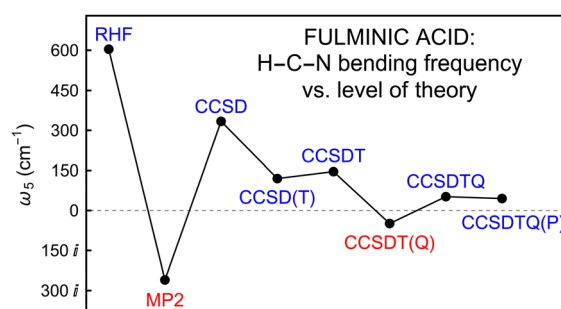
Marie Pinto, Maryam Saliminasab, Andrew Harris, Michalis Lazaratos, Ana-Nicoleta Bondar, Vladimir Ladizhansky* and Leonid S. Brown*



24109

Fulminic acid: a quasibent spectacle

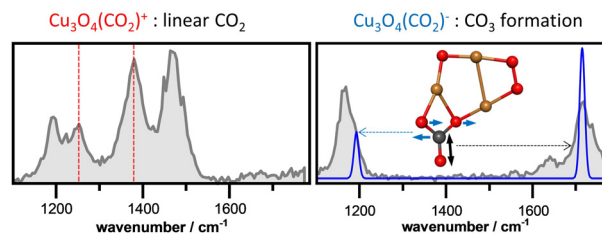
Ashley M. Allen, Laura N. Olive, Patricia A. Gonzalez Franco, Shiblee R. Barua, Wesley D. Allen and Henry F. Schaefer III*



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CO₂ activation by copper oxide clusters: size, composition, and charge state dependence

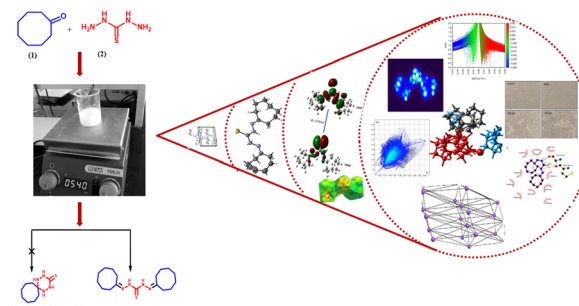
Pavol Mikolaj, Barbara Zamora Yusti, László Nyulászi, Joost M. Bakker, Tibor Höltzl* and Sandra M. Lang*



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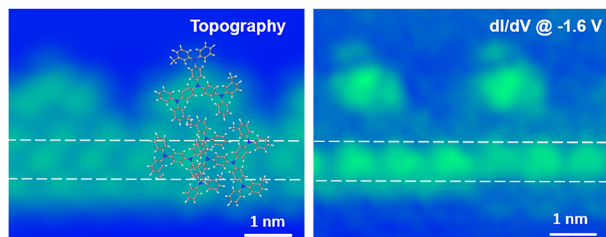
Synthesis, crystal structure analysis, computational modelling and evaluation of anti-cervical cancer activity of novel 1,5-dicyclooctyl thiocarbohydrazone

Soni Shukla, Prince Trivedi, Delna Johnson, Pulkit Sharma, Abhinav Jha, Habiba Khan, Vijay Thiruvengatam, Monisha Banerjee and Abha Bishnoi*



RESEARCH PAPERS

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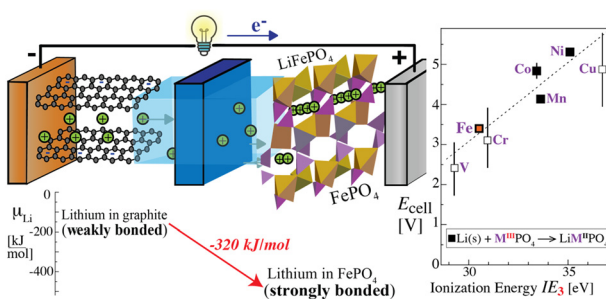


Characteristic “plug-in” configuration of SBM on Au(111) with 1D electronic state

Exploring the characteristic “plug-in” configuration of an adsorbed starburst molecule

Xiaoyu Hao, Yan Li, Teng Zhang,* Mengmeng Niu, Huixia Yang, Jingsi Qiao, Cesare Grazioli, Ambra Guarnaccio, Liwei Liu, Quanzhen Zhang,* Carla Puglia and Yeliang Wang*

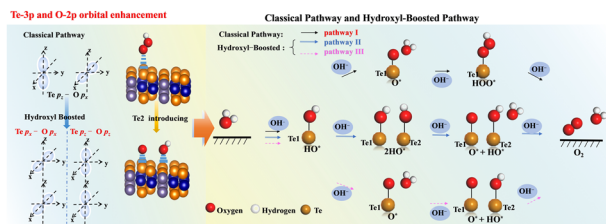
24157



How lithium-ion batteries work conceptually: thermodynamics of Li bonding in idealized electrodes

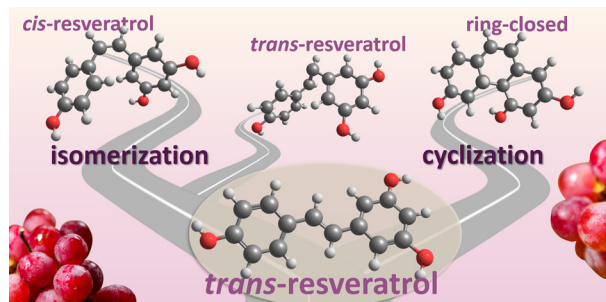
Sam H. Finkelstein, Marco Ricci, Tom Böttcher and Klaus Schmidt-Rohr*

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Enhanced oxygen evolution reaction activity on two-dimensional vdW ferromagnetic Cr₂Ge₂Te₆ through synergism between two active sites

Zongxiang Kang, Wei Su, Qihong Li, Jingguo Hu and Jing Pan*

24179

Photoisomerization pathways of *trans*-resveratrol

Mariana Yoshinaga, Josene M. Toldo, Willian R. Rocha* and Mario Barbatti*



CORRECTION

24189

Correction: Novel germanene–arsenene and germanene–antimonene lateral heterostructures: interline-dependent electronic and magnetic properties

Chu Viet Ha, Bich Ngoc Nguyen Thi, Pham Quynh Trang, R. Ponce-Pérez, J. Guerrero-Sanchez and D. M. Hoat*

