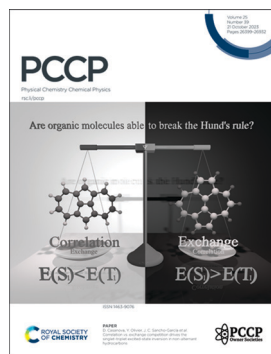


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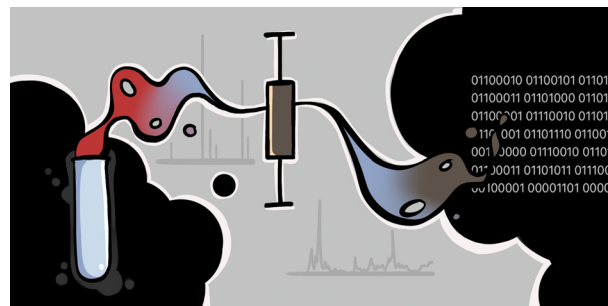
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EDITORIAL

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Benchmark experiments for numerical quantum chemistry

Ricardo A. Mata, Anne Zehnacker-Rentien and Martin A. Suhm

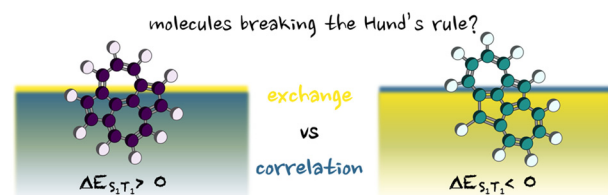


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Correlation vs. exchange competition drives the singlet–triplet excited-state inversion in non-alternant hydrocarbons

M. E. Sandoval-Salinas, G. Ricci, A. J. Pérez-Jiménez, D. Casanova,* Y. Olivier* and J. C. Sancho-García*



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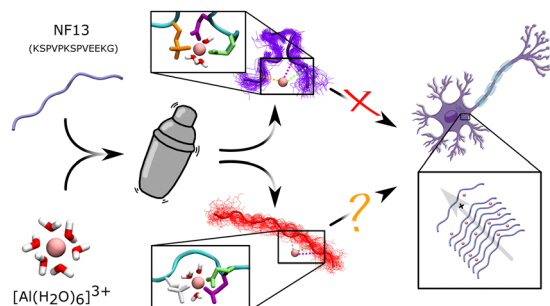


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Influence of metal binding on the conformational landscape of neurofilament peptides

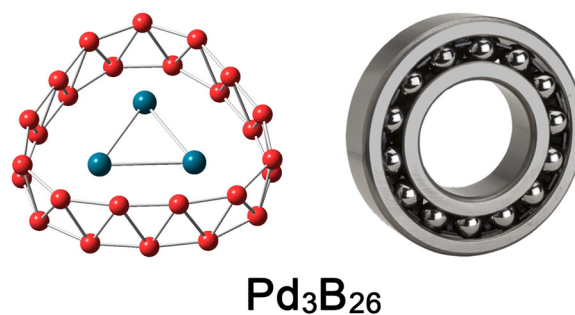
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Boron-based Pd₃B₂₆ alloy cluster as a nanoscale antifriction bearing system: tubular core-shell structure, double π/σ aromaticity, and dynamic structural fluxionality

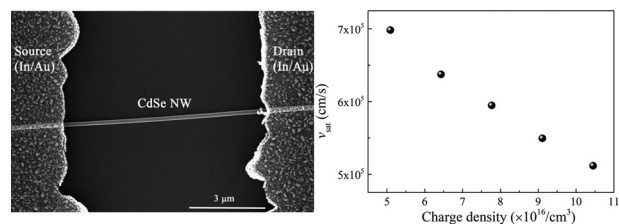
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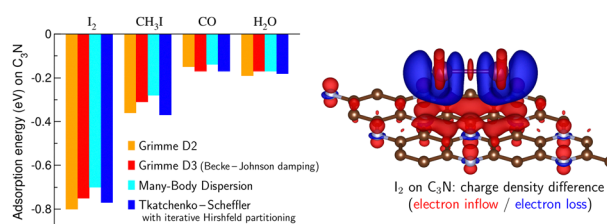
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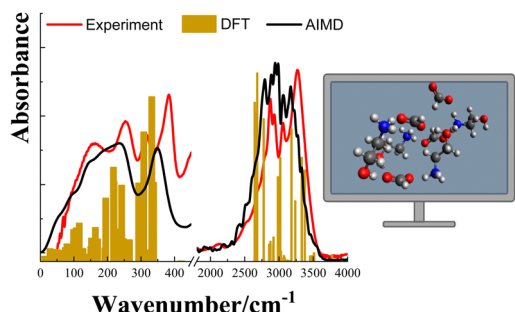
Potential of nanostructured carbon materials for iodine detection in realistic environments revealed by first-principles calculations

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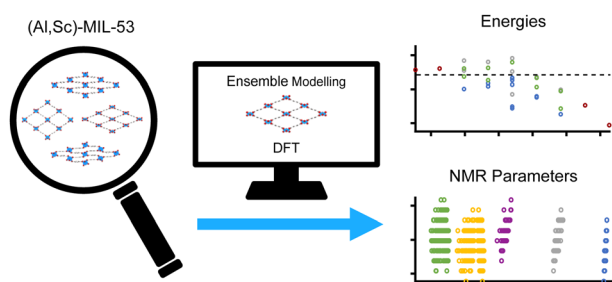
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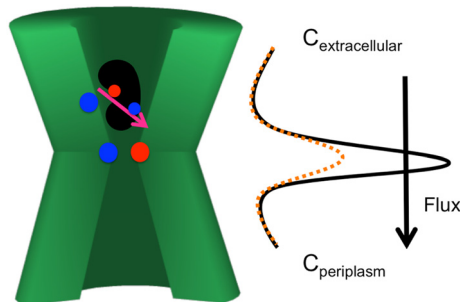
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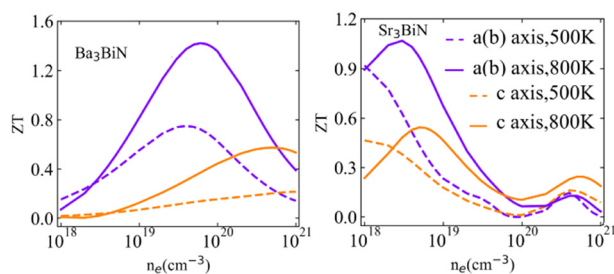
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The mechanism of an electrostatic nanofilter: overcoming entropy with electrostatics

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Shuming Zeng,* Xiang Yan, Qian Shen, Yusong Tu, Hao Huang* and Geng Li*

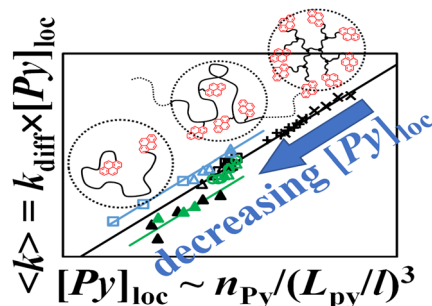


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Probing the inner local density of complex macromolecules by pyrene excimer formation

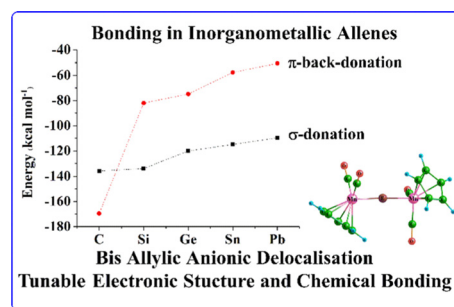
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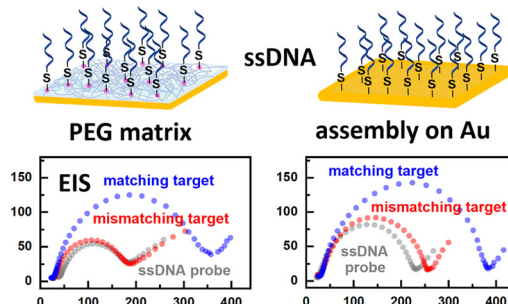
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Exploiting epoxy-rich poly(ethylene glycol) films for highly selective ssDNA sensing via electrochemical impedance spectroscopy

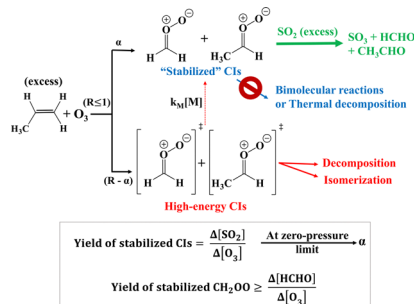
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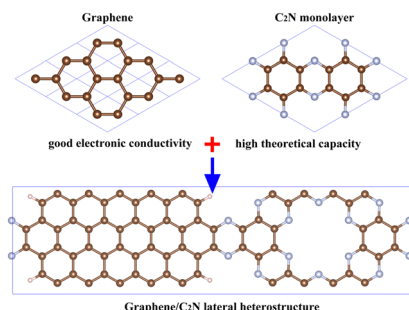
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Yawen Chen, Qianru Wang, Quan Zhang, Shengli Zhang and Yang Zhang*

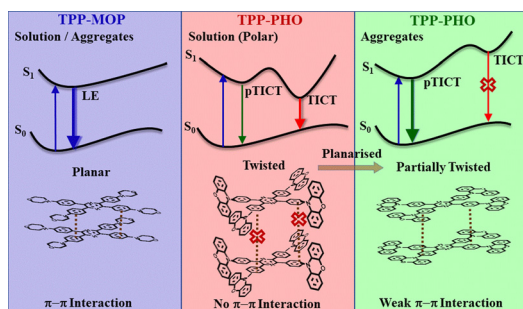
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Min Zhao, Weizhen Meng,* Lirong Wang, Zeqing He, Lei Jin, Ying Liu, Xuefang Dai, Xiaoming Zhang,* Hongshi Li* and Guodong Liu*

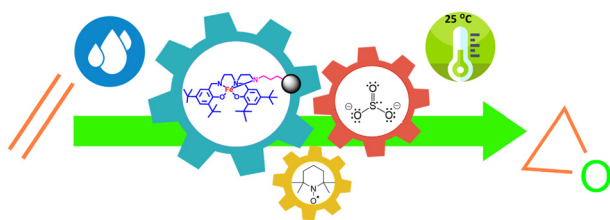
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Molecular torsion controls the excited state relaxation pathways of multibranched tetraphenylpyrazines: effect of substitution of morpholine vs. phenoxazine

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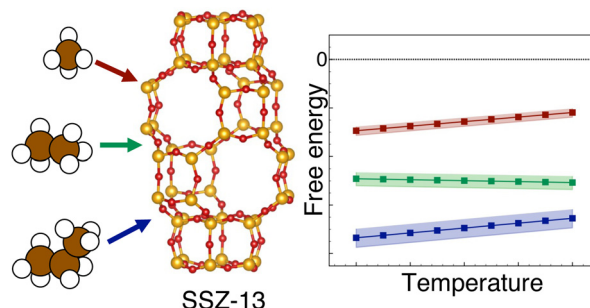


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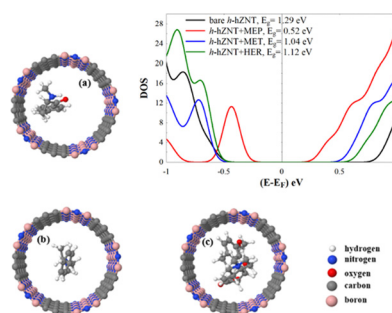
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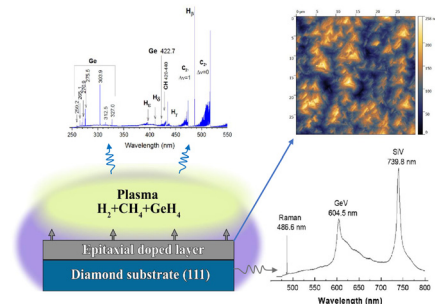
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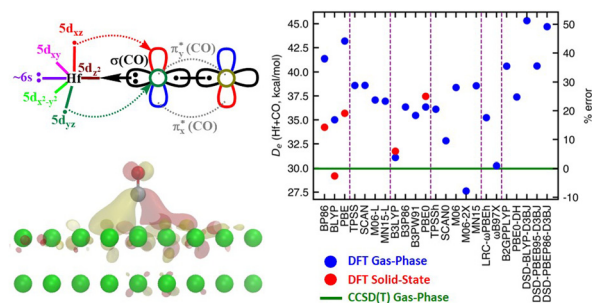
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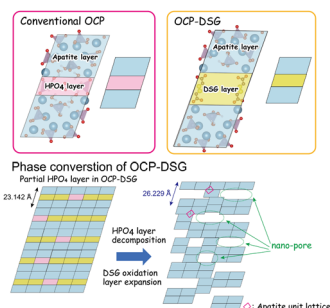
Gas-phase and solid-state electronic structure analysis and DFT benchmarking of HfCO

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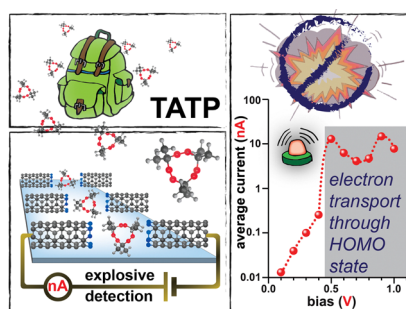
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Interlayer expansion of octacalcium phosphate via forced oxidation of the intercalated molecules within its interlayers

Yuki Sugiura,* Etsuko Yamada and Masanori Horie

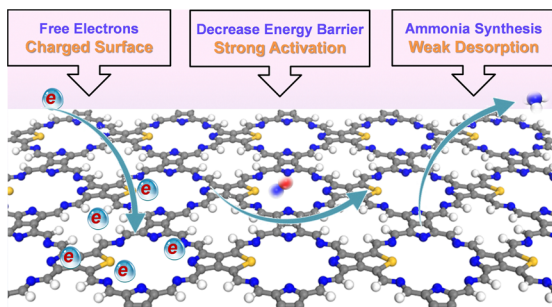
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Aleksandar Ž. Tomović, Helena Miljkovic, Miloš S. Dražić, Vladimir P. Jovanović and Radomir Zikic*

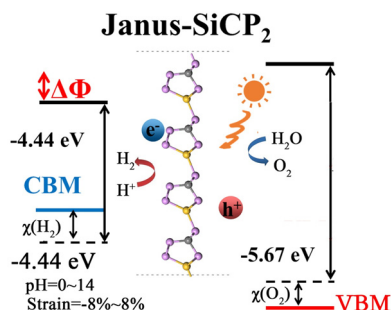
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Lei Yang, Jiake Fan and Weihua Zhu*

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Metal-free Janus α - and β -SiCP₄: designing stable and efficient two-dimensional semiconductors for water splitting

Yanfu Zhao, Bofeng Zhang* and Jiahe Lin*

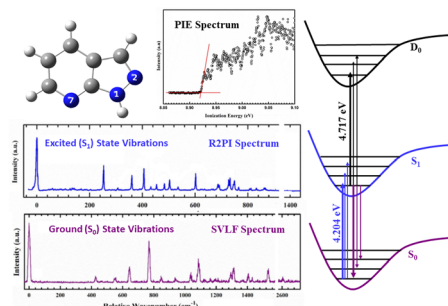


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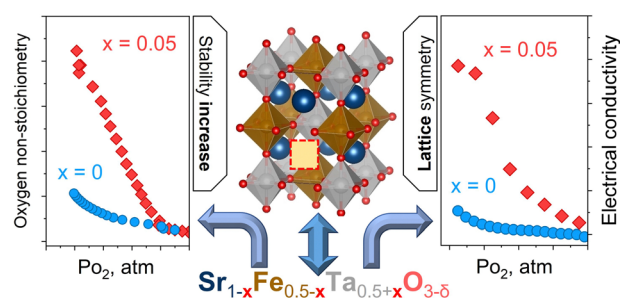
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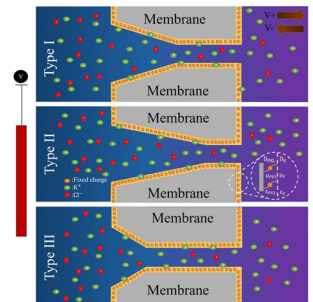
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Smart nanochannels: tailoring ion transport properties through variation in nanochannel geometry

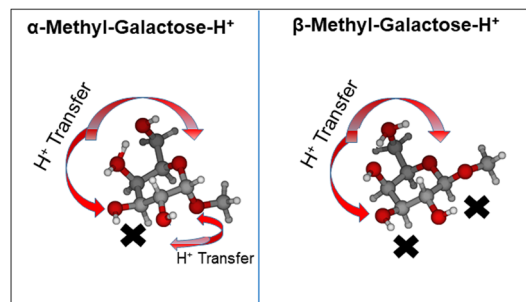
Amirhossein Heydari, Mahdi Khatibi and Seyed Nezameddin Ashrafizadeh*



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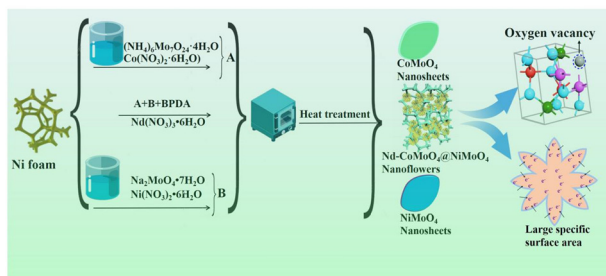
Selective reactivity of glycosyl cation stereoisomers: the role of intramolecular hydrogen bonding

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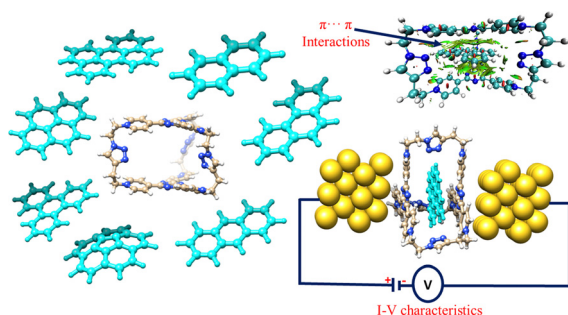
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Coupling of Nd doping and oxygen-rich vacancy in CoMoO₄@NiMoO₄ nanoflowers toward advanced supercapacitors and photocatalytic degradation

Jing Wang,* Gang Wang, Shen Wang, Tingting Hao and Jian Hao

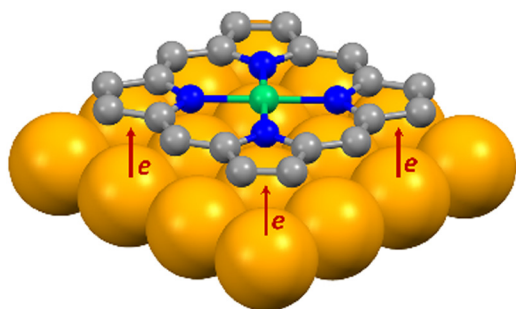
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Exploring π – π interactions and electron transport in complexes involving a hexacationic host and PAH guest: a promising avenue for molecular devices

Haobam Kisan Singh, Upasana Nath, Niharika Keot and Manabendra Sarma*

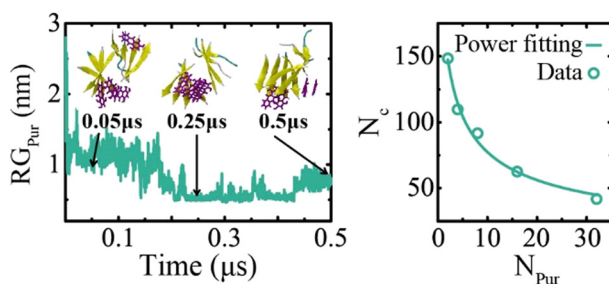
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A local point of view of the Cu(100) \rightarrow NiTPP charge transfer at the NiTPP/Cu(100) interface

Silvia Carlotto, Alberto Verdini,* Giovanni Zamborlini, Iulia Cojocariu, Vitaliy Feyrer, Luca Floreano and Maurizio Casarin*

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Dose-dependent binding behavior of anthraquinone derivative purpurin interacting with tau-derived peptide protofibril

Xiaoxiao Wu, Lili Zhu, Gang Wang, Qingwen Zhang and Zhenyu Qian*

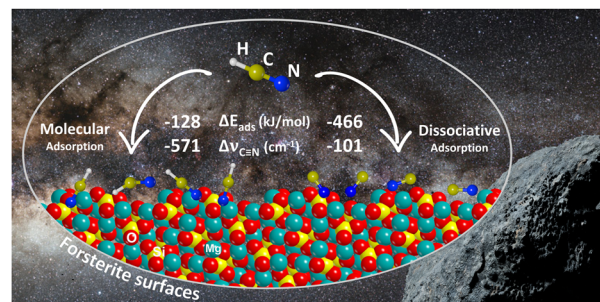


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Adsorption of HCN on cosmic silicates: a periodic quantum mechanical study

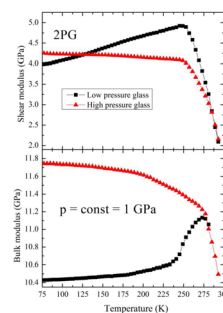
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Thermobaric history as a tool to govern properties of glasses: case of dipropylene glycol

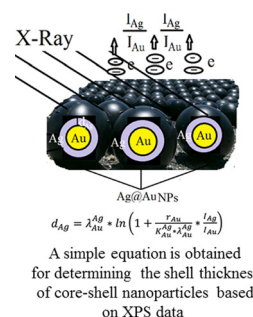
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A simple equation to determine the shell thicknesses of core-shell nanoparticles based on XPS data of their elemental composition

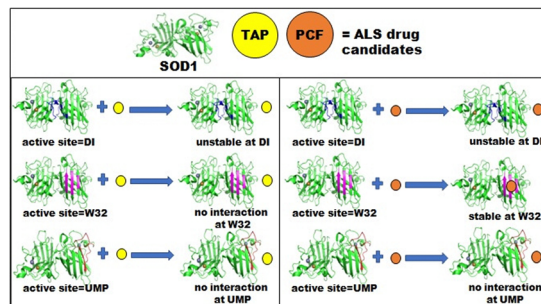
Alexey T. Kozakov,* Anton A. Skriabin and Niranjana Kumar



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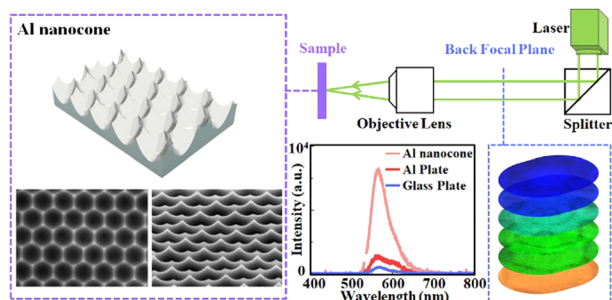
In silico analysis of SOD1 aggregation inhibition modes of tertiary amine pyrazolone and pyrano coumarin ferulate as ALS drug candidates

Aziza Rahman, Bondeepa Saikia and Anupaul Baruah*



RESEARCH PAPERS

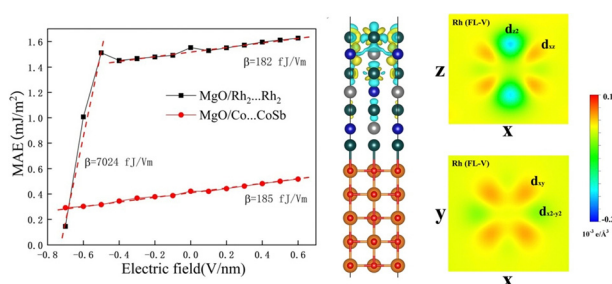
26847



Surface lattice resonances enhanced directional amplified spontaneous emission on plasmonic honeycomb nanocone array

Dongda Wu, Yi Wang,* Jiamin Xiao, Jiang Hu, Xuchao Zhao, Yuhao Gao, Jiazhi Yuan and Wenxin Wang*

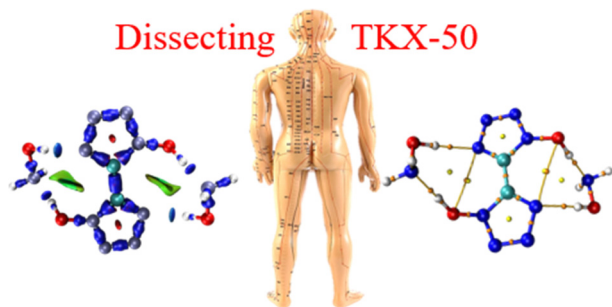
26853



Giant unilateral electric-field control of magnetic anisotropy in MgO/Rh₂CoSb heterojunctions

Shiming Yan, Yue Hu, Deyou Jin, Ru Bai, Wen Qiao* and Tiejun Zhou*

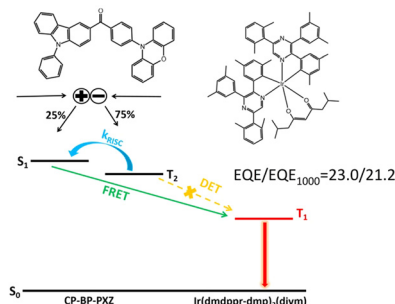
26861



Theoretical study on intra-molecule interactions in TKX-50

Chunhai Yang,* Xue Li,* Ning Zhou, Huilong Dong,* Xiuli Hu, Junxun Jin, Tao Huang and Jinhui Wang

26878



Exciton dynamics of an aggregation-induced delayed fluorescence emitter in non-doped OLEDs and its application as host for high-efficiency red phosphorescent OLEDs

Hanlin Li, Chengwei Lin, Yibing Wu, Xianfeng Qiao, Dezhi Yang, Yanfeng Dai, Qian Sun, Tansir Ahamad, Zhuji Zhao* and Dongge Ma*

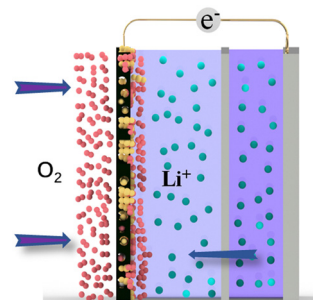


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26885

Cobalt-doped tin disulfide catalysts for high-capacity lithium–air batteries with high lifetime

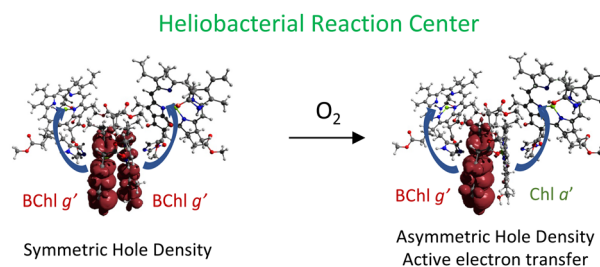
Jie Li, Yuzhi Shi, Junhai Wang, Qianhe Liu, Lihua Luan, Qiang Li, Qinghao Cao, Tianyu Zhang and Hong Sun*



26894

Electronic structure and energetics of a heterodimeric BChl *g'*/Chl *a'* special pair generated by exposure of *Heliomicrobium modesticaldum* to dioxygen

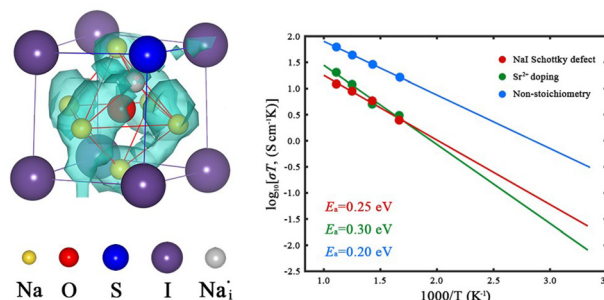
Divya Kaur,* Bryan Ferlez, Patrick Landry, Till Biskup, Stefan Weber, John H. Golbeck,* K. V. Lakshmi* and Art van der Est*



26906

Investigation of the sodium-ion transport mechanism and elastic properties of double anti-perovskite Na₃S_{0.5}O_{0.5}I

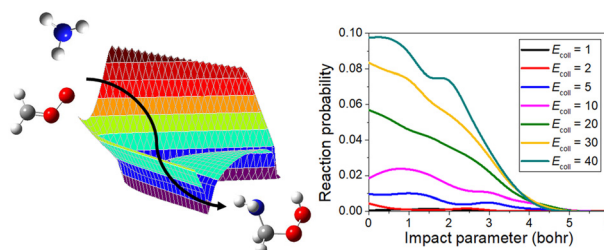
Sen Lian, Congcong Li, Chen Kang, Junfeng Ren and Meina Chen*



26917

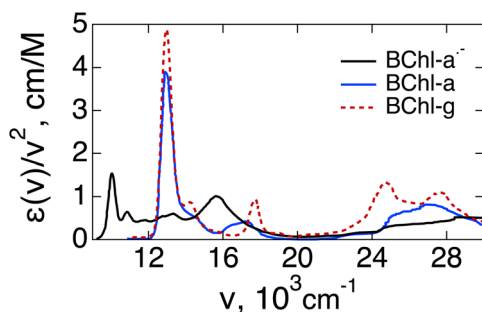
Full-dimensional automated potential energy surface development and detailed dynamics for the CH₂OO + NH₃ reaction

Cangtao Yin* and Gábor Czako*



COMMENT

26923



Comment on “Applicability of perturbed matrix method for charge transfer studies at bio/metallic interfaces: a case of azurin” by O. Kontkanen, D. Biriukov and Z. Futera, *Phys. Chem. Chem. Phys.*, 2023, 25, 12479

Setare Mostajabi Sarhangi and Dmitry V. Matyushov*

CORRECTION

26929

Correction: Induced UV photon sensing properties in narrow bandgap CdTe quantum dots through controlling hot electron dynamics

Thankappan Thrupthika, Devaraj Nataraj,* Subramaniam Ramya, Arumugam Sangeetha and T. Daniel Thangadurai

