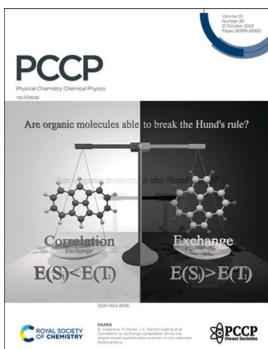


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See D. Casanova, Y. Olivier, J. C. Sancho-Garcia et al., pp. 26417–26428.
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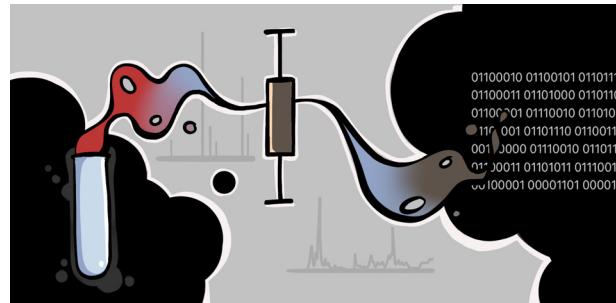
See David de Sancho, Xabier Lopez et al., pp. 26429–26442.
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Correlation vs. exchange competition drives the singlet–triplet excited-state inversion in non-alternant hydrocarbons

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



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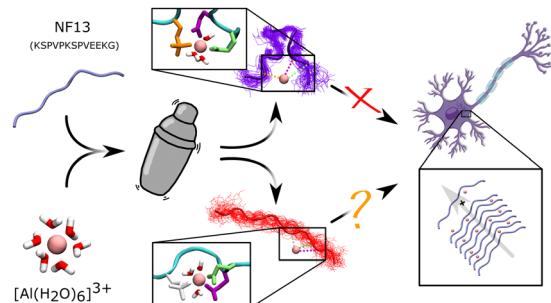


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Influence of metal binding on the conformational landscape of neurofilament peptides

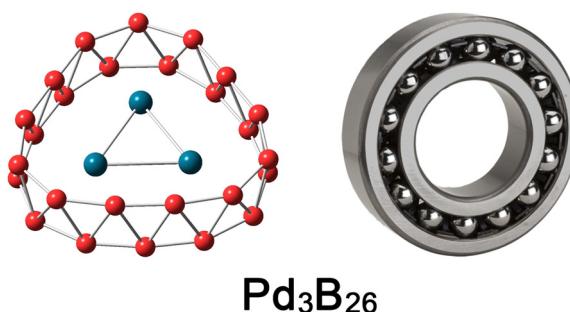
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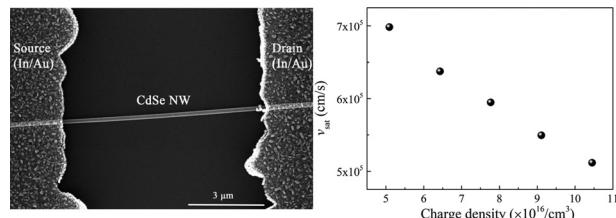
Lin-Yan Feng, Jin-Chang Guo, Ying-Jin Wang, Xiao-Ying Zhang and Hua-Jin Zhai*



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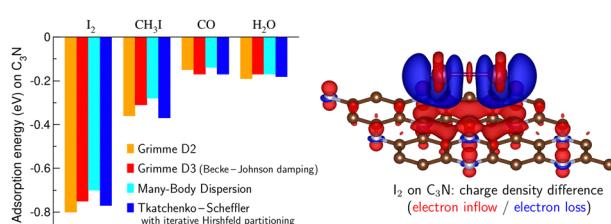
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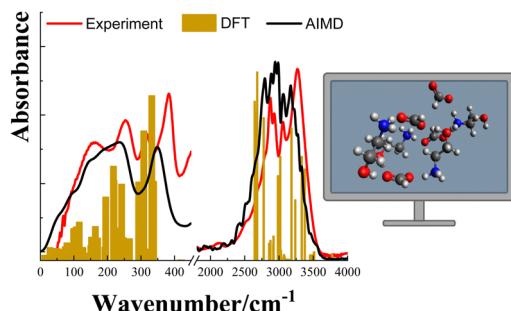
Potential of nanostructured carbon materials for iodine detection in realistic environments revealed by first-principles calculations

Kazem Zhour, Ayoub Daouli, Andrei Postnikov,* Abdellatif Hasnaoui and Michael Badawi*



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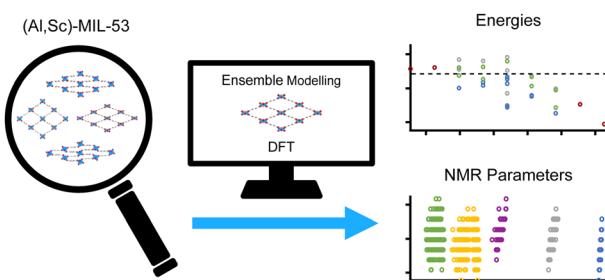
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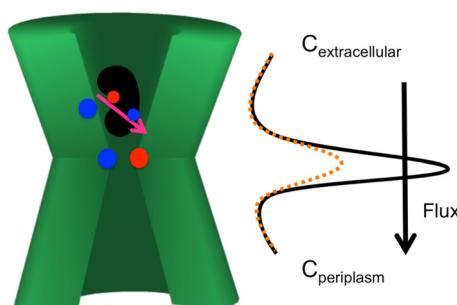
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Zachary H. Davis, Emma A. L. Borthwick, Russell E. Morris* and Sharon E. Ashbrook*

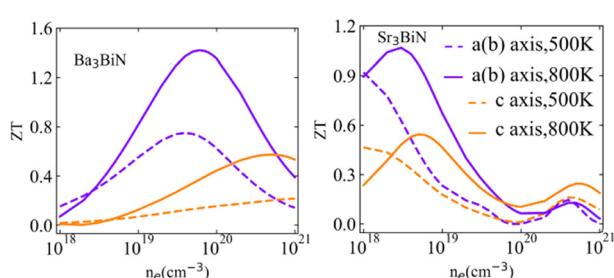
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Igor Bodrenko, Matteo Ceccarelli* and Silvia Acosta-Gutierrez

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

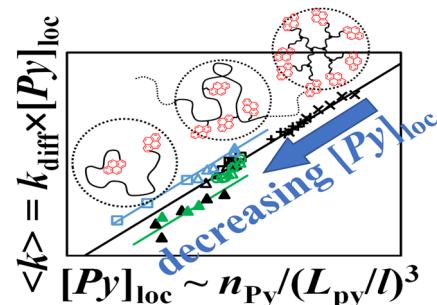


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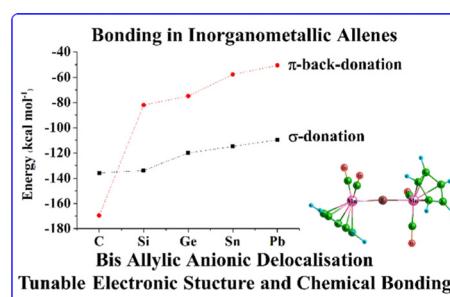
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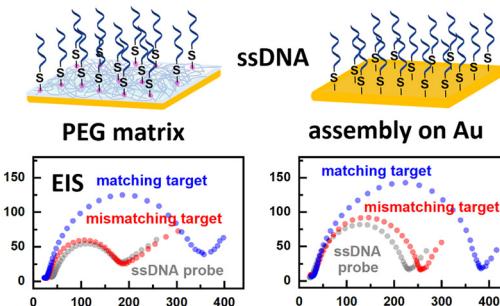
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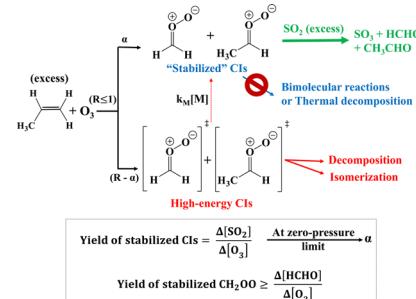
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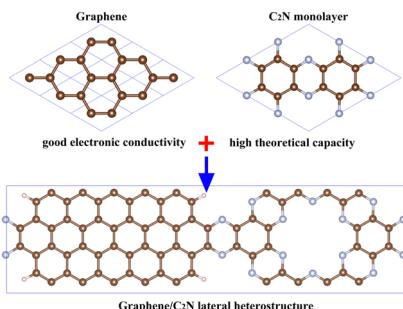
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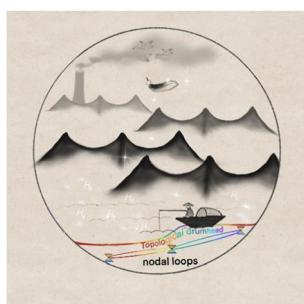
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**Graphene/C₂N lateral heterostructures as promising anode materials for lithium-ion batteries**

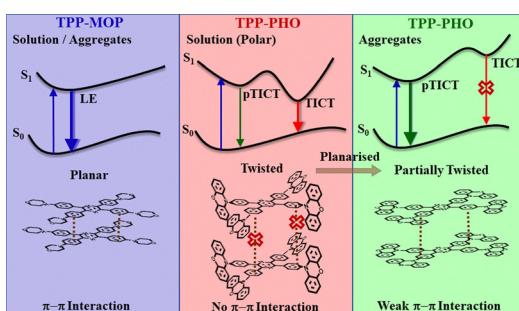
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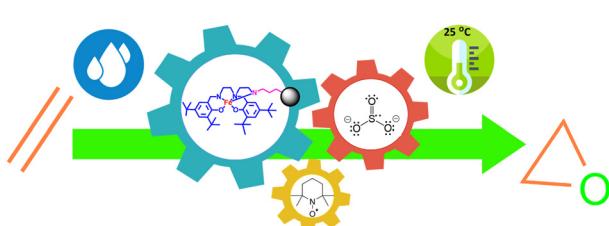
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Pegah Mohammadpour, Elham Safaei,* Elham Mazarei and Constantinos D. Zeinalipour-Yazdi

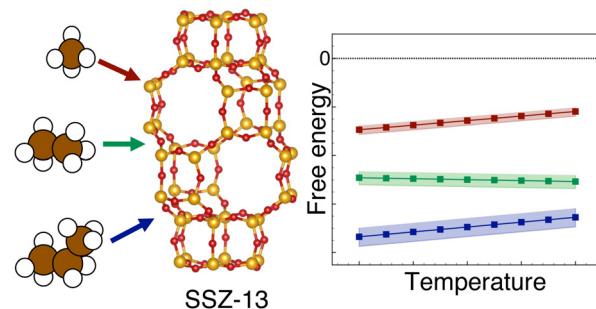


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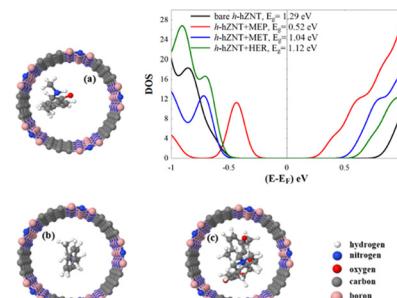
Free and internal energies for the adsorption of short alkanes into the zeolite SSZ-13 from *ab initio* molecular dynamics simulations

Daniel J. Hutton and Florian Göltl*



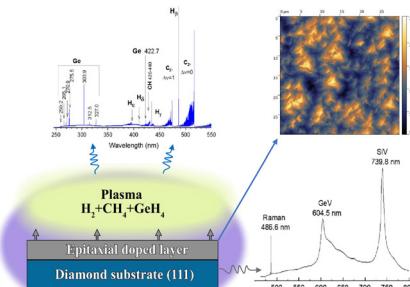
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Towards nanotube-based sensors for discrimination of drug molecules

Laith A. Algharagholy, Víctor M. García-Suárez,*
Ohood Abdullah Albeydani and Jehan Alqahtani

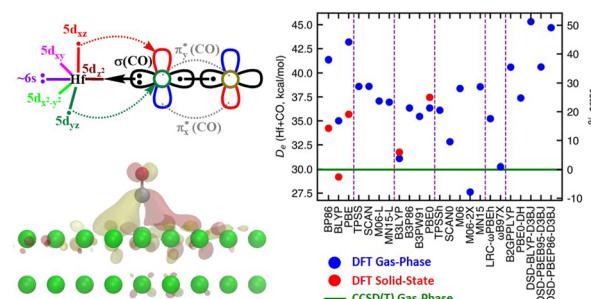
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***In situ* doping of epitaxial diamond with germanium by microwave plasma CVD in $\text{GeH}_4\text{-CH}_4\text{-H}_2$ mixtures with optical emission spectroscopy monitoring**

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Irina Fedorova, Artem Martyanov, Pavel Pivovarov,
Vladimir Artemov, Andrew Khomich, Roman Khmelnitskiy
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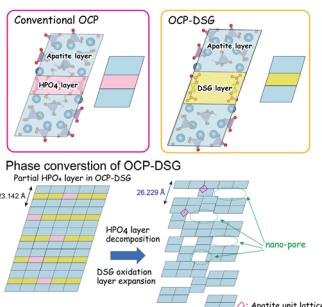
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Gas-phase and solid-state electronic structure analysis and DFT benchmarking of HfCO

Isuru R. Ariyarathna, Yeongsu Cho, Chenru Duan and
Heather J. Kulik*

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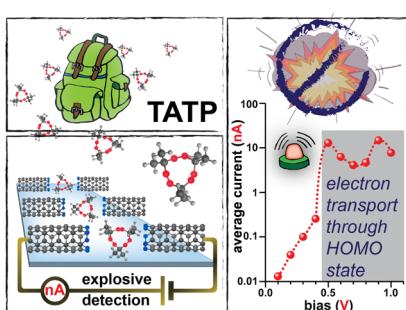
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Interlayer expansion of octacalcium phosphate via forced oxidation of the intercalated molecules within its interlayers

Yuki Sugiura,* Etsuko Yamada and Masanori Horie

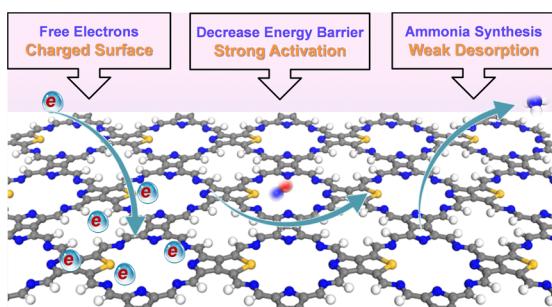
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Tunnel junction sensing of TATP explosive at the single-molecule level

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

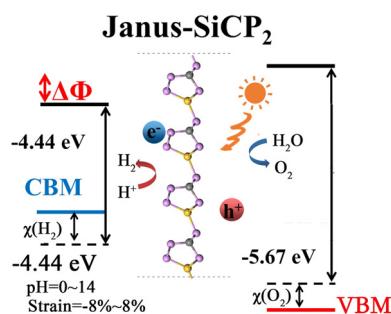
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Theoretical insight into the essential role of charged surface for ammonia synthesis: Si-decorated carbon nitride electrode

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*

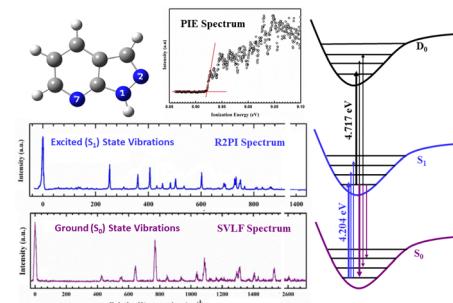


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Laser spectroscopic characterization of supersonic jet cooled 2,7-diazaindole

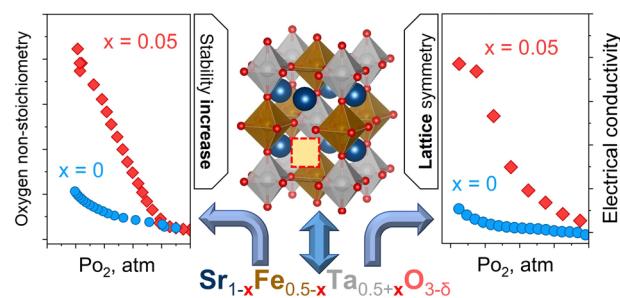
Simran Baweja, Bhavika Kalal and Surajit Maity*



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The influence of strontium deficiency on thermodynamics of defect formation, structural stability and electrical transport of $\text{SrFe}_{0.5}\text{Ta}_{0.5}\text{O}_{3-\delta}$ -based solid solutions with an excess tantalum content

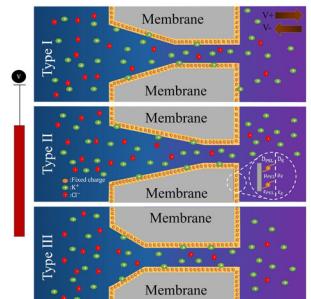
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Smart nanochannels: tailoring ion transport properties through variation in nanochannel geometry

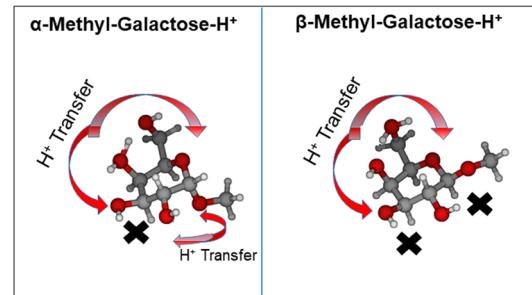
Amirhossein Heydari, Mahdi Khatibi and Seyed Nezameddin Ashrafizadeh*



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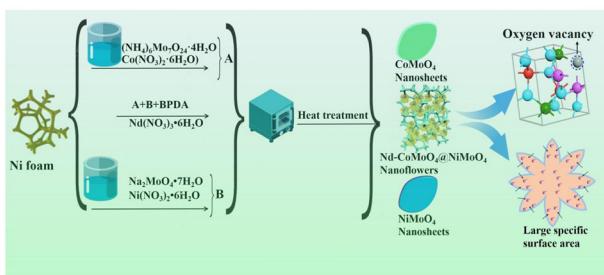
Selective reactivity of glycosyl cation stereoisomers: the role of intramolecular hydrogen bonding

M. P. Dvores,* P. Çarçabal and R. B. Gerber*



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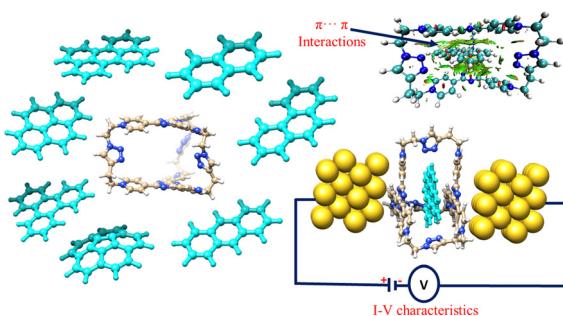
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Coupling of Nd doping and oxygen-rich vacancy in $\text{CoMoO}_4@\text{NiMoO}_4$ nanoflowers toward advanced supercapacitors and photocatalytic degradation

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

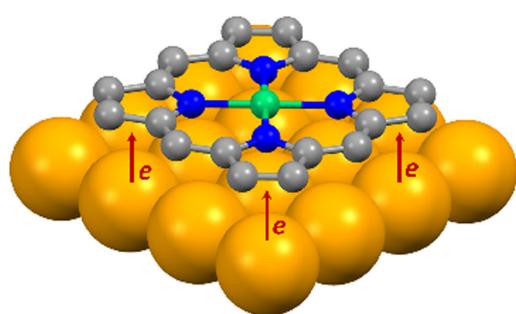
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Exploring $\pi-\pi$ interactions and electron transport in complexes involving a hexacationic host and PAH guest: a promising avenue for molecular devices

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

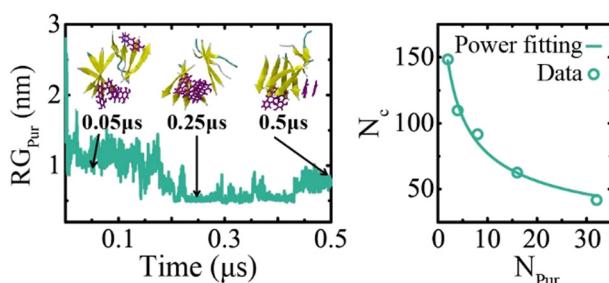
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A local point of view of the $\text{Cu}(100) \rightarrow \text{NiTPP}$ charge transfer at the NiTPP/Cu(100) interface

Silvia Carlotto, Alberto Verdini,* Giovanni Zamborlini, Iulia Cojocariu, Vitaliy Feyer, 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*

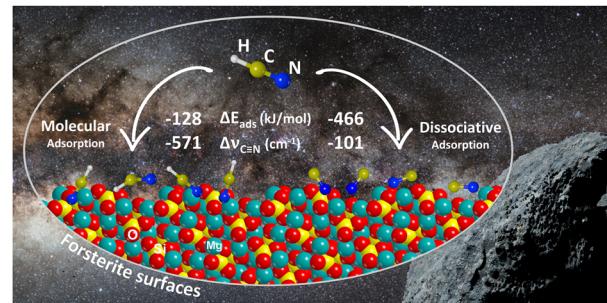


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Adsorption of HCN on cosmic silicates: a periodic quantum mechanical study

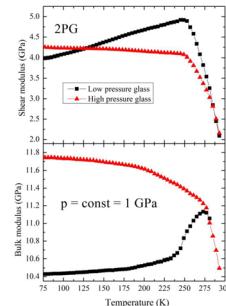
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Thermobaric history as a tool to govern properties of glasses: case of dipropylene glycol

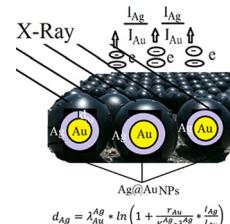
Igor Danilov,* Elena Gromnitskaya and Vadim Brazhkin



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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 Niranjan Kumar

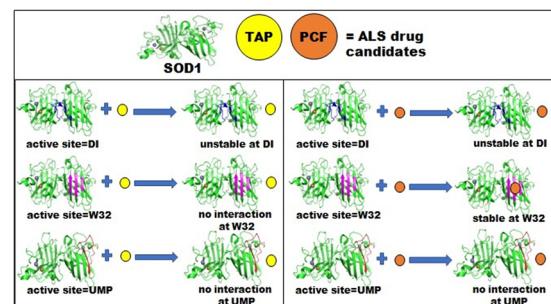


A simple equation is obtained for determining the shell thickness of core–shell nanoparticles based on XPS data

26833

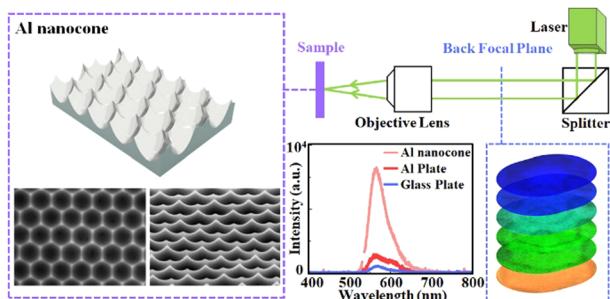
***In silico* analysis of SOD1 aggregation inhibition modes of tertiary amine pyrazolone and pyrano coumarin ferulate as ALS drug candidates**

Aziza Rahman, Bondeepa Saikia and Anupaul Baruah*



RESEARCH PAPERS

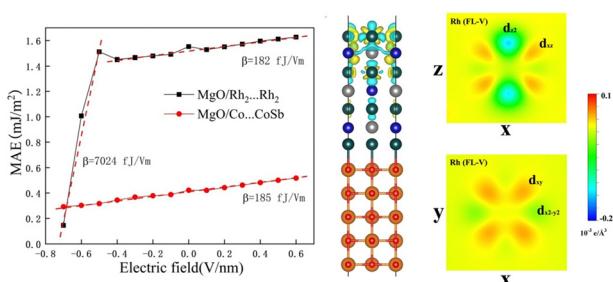
26847



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*

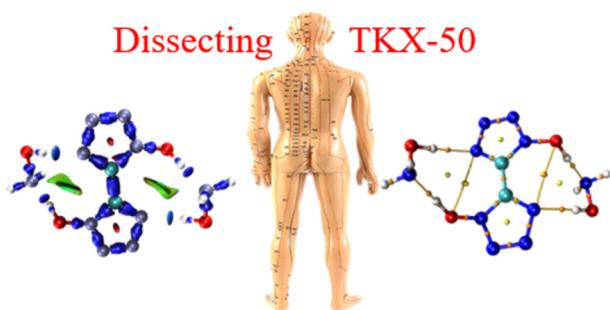
26853



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*

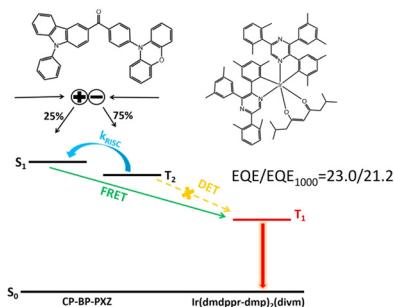
26861



Theoretical study on intra-molecule interactions in TKX-50

Chunhai Yang,* Xue Li,* Ning Zhou, Hui long 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, Zhujin Zhao* and Dongge Ma*

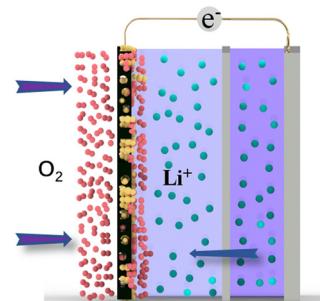


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26885

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

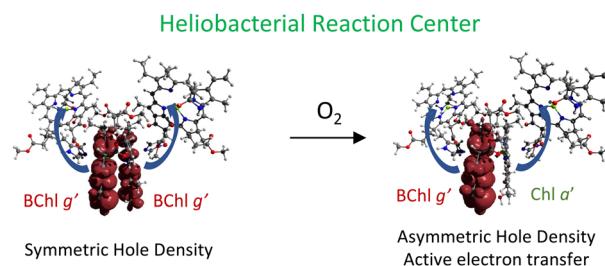
Jie Li, Yuzhi Shi, Junhai Wang, Qianhe Liu, Lihua Luan, Qiang Li, Qinghao Cao, Tianyu Zhang and Hong Sun*



26894

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

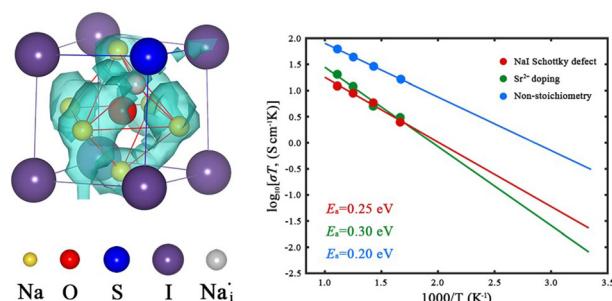
Divya Kaur,* Bryan Ferlez, Patrick Landry, Till Biskup, Stefan Weber, John H. Golbeck,* K. V. Lakshmi* and Art van der Est*



26906

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

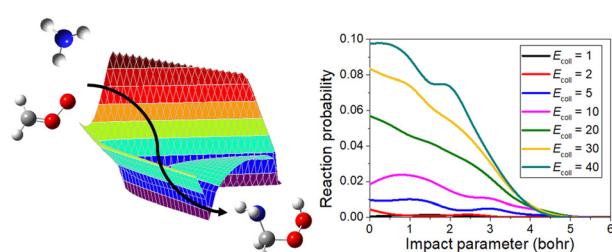
Sen Lian, Congcong Li, Chen Kang, Junfeng Ren and Meina Chen*



26917

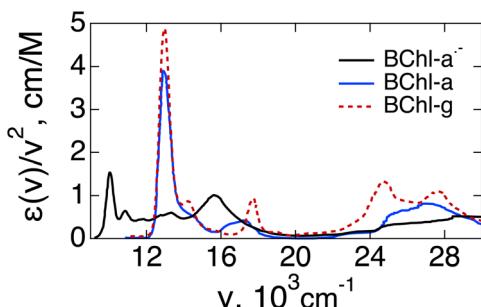
Full-dimensional automated potential energy surface development and detailed dynamics for the CH₂OO + NH₃ reaction

Cangtao Yin* and Gábor Czakó*



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