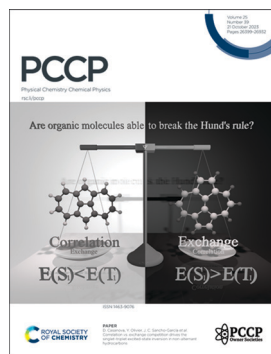


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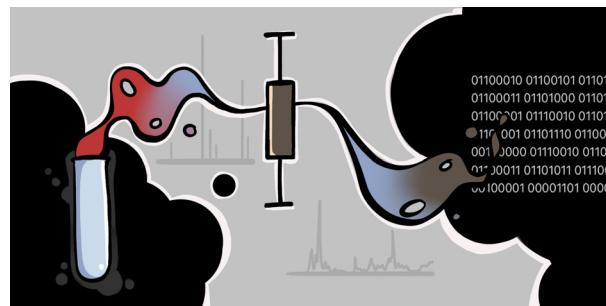
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EDITORIAL

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Benchmark experiments for numerical quantum chemistry

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

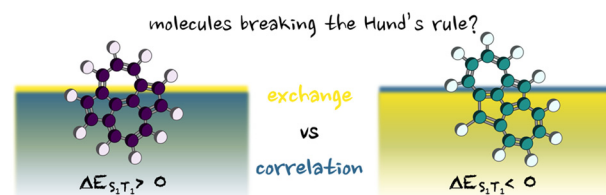


RESEARCH PAPERS

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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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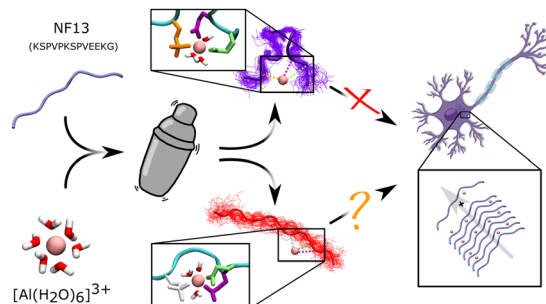


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Influence of metal binding on the conformational landscape of neurofilament peptides

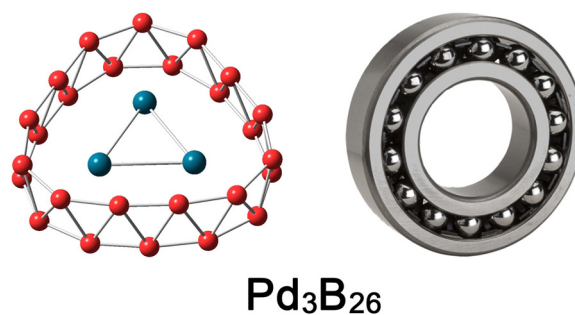
David Silva-Brea, David de Sancho* and Xabier Lopez*



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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

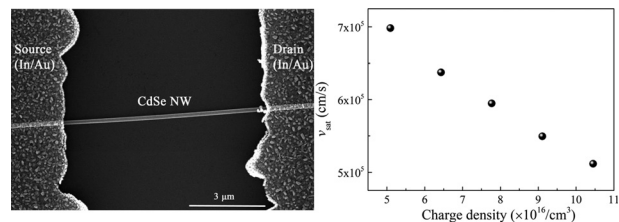
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Drift velocity saturation in field-effect transistors based on single CdSe nanowires

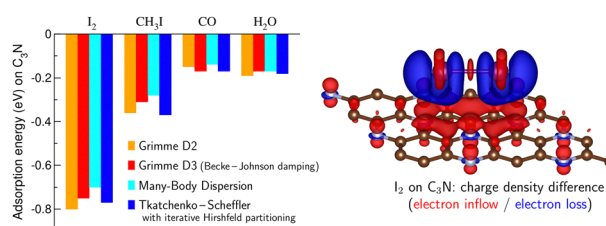
Weifeng Jin* and Xinyang Yang



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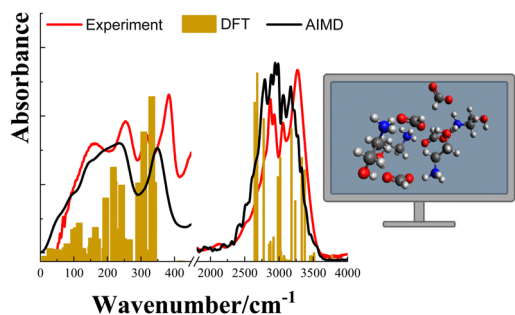
Potential of nanostructured carbon materials for iodine detection in realistic environments revealed by first-principles calculations

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



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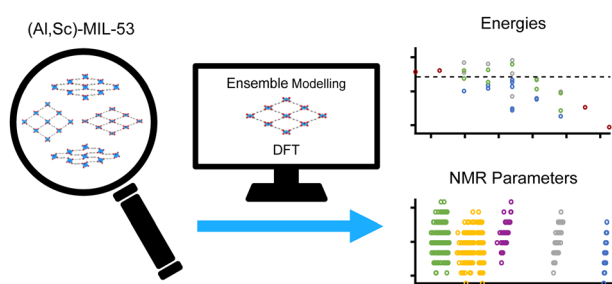
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DFT and *ab initio* molecular dynamics simulation study of the infrared spectrum of the protic ionic liquid 2-hydroxyethylammonium formate

Vitor Hugo Paschoal and Mauro C. C. Ribeiro*

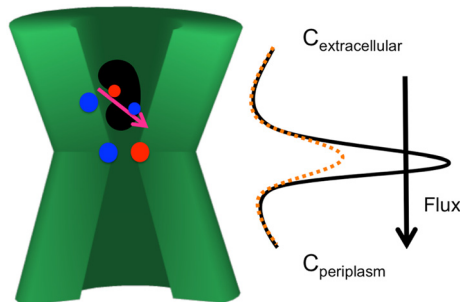
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Computational NMR investigation of mixed-metal (Al,Sc)-MIL-53 and its phase transitions

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

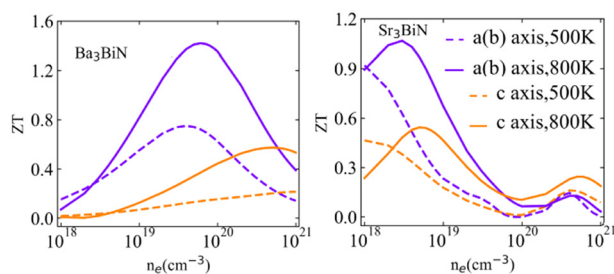
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The mechanism of an electrostatic nanofilter: overcoming entropy with electrostatics

Igor Bodrenko, Matteo Ceccarelli* and Silvia Acosta-Gutierrez

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Low lattice thermal conductivities and good thermoelectric performance of hexagonal antiperovskites X(Ba & Sr)₃BiN with quartic anharmonicity

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

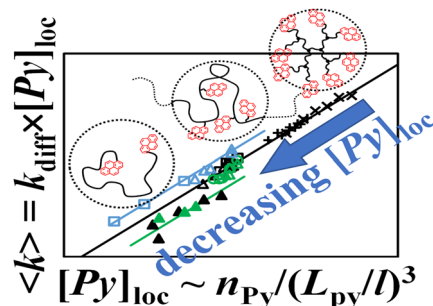


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Probing the inner local density of complex macromolecules by pyrene excimer formation

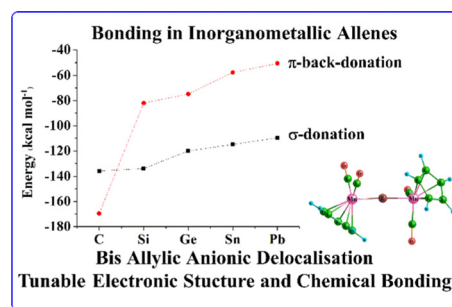
Hunter Little, Sanjay Patel and Jean Duhamel*



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Inorganometallic allenes [(Mn(η^5 -C₅H₅)(CO)₂)₂(μ -E)] (E = Si–Pb): bis-allylic anionic delocalisation similar to organometallic allene but differential σ -donation and π -backdonation

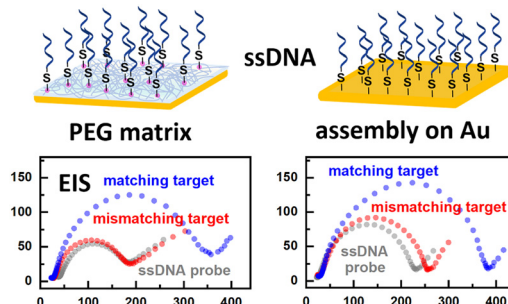
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Exploiting epoxy-rich poly(ethylene glycol) films for highly selective ssDNA sensing via electrochemical impedance spectroscopy

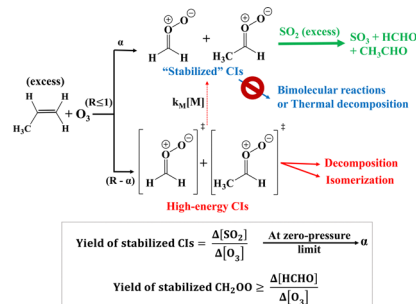
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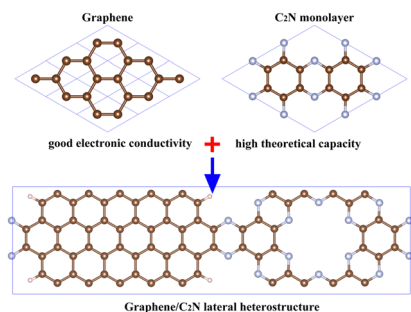
Low-pressure and nascent yields of stabilized Criegee intermediates CH₂OO and CH₃CHOO in ozonolysis of propene

Lei Yang, Mixtli Campos-Pineda, Katia Hatem and Jingsong Zhang*



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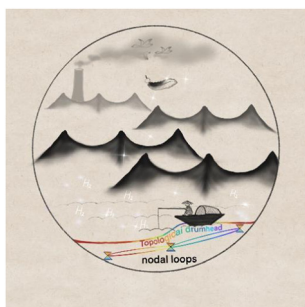
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Graphene/C₂N lateral heterostructures as promising anode materials for lithium-ion batteries

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

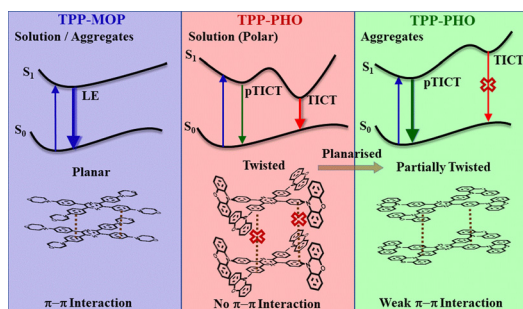
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Drumhead surface states promoted hydrogen evolution reactions in type-II nodal-line topological catalyst Mg₃Bi₂

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

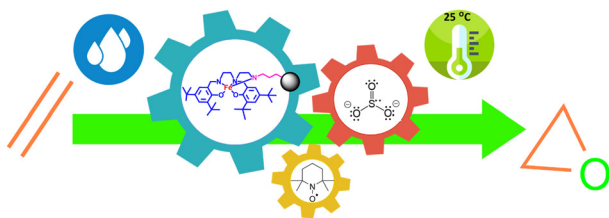
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Molecular torsion controls the excited state relaxation pathways of multibranch tetraphenylpyrazines: effect of substitution of morpholine vs. phenoxazine

Hasim Fayiz Pananilath, Chinju Govind, Tessa D. Thadathilanickal and Venugopal Karunakaran*

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TEMPO and a co-reductant mediated aerobic epoxidation of olefins using a new magnetically recoverable iron(III) bis(phenol)diamine complex: experimental and computational studies

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

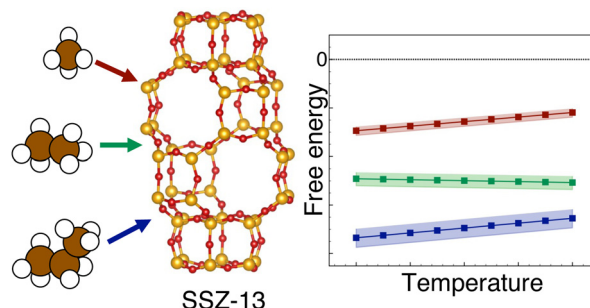


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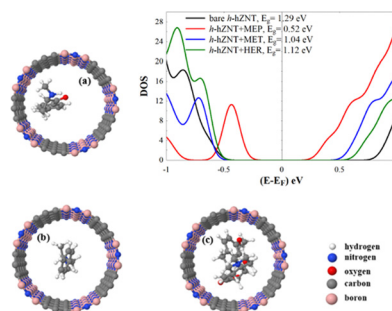
Free and internal energies for the adsorption of short alkanes into the zeolite SSZ-13 from *ab initio* molecular dynamics simulations

Daniel J. Hutton and Florian Göttl*

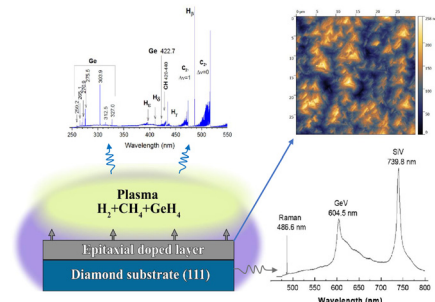


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Towards nanotube-based sensors for discrimination of drug molecules

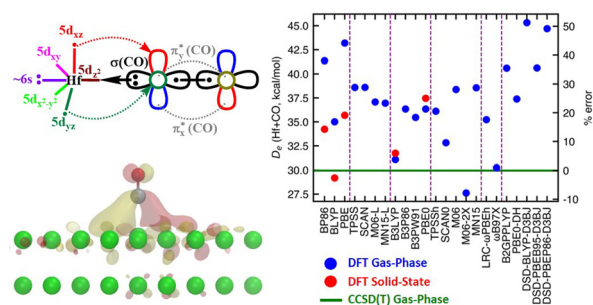
Laith A. Algharagholy, Víctor M. García-Suárez,*
Ohood Abdullah Albeydani and Jehan Alqahtani

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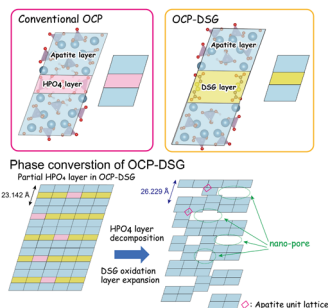
In situ doping of epitaxial diamond with germanium by microwave plasma CVD in GeH₄-CH₄-H₂ mixtures with optical emission spectroscopy monitoringVladimir Yurov,* Andrey Bolshakov, Victor Ralchenko,*
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Vladimir Artemov, Andrew Khomich, Roman Khmelnskiy
and Kirill Boldyrev

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

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

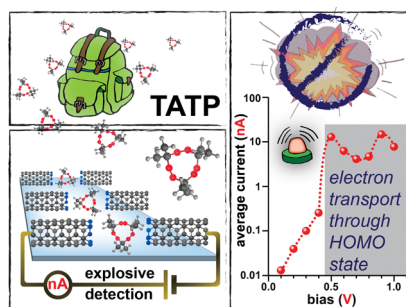
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Interlayer expansion of octacalcium phosphate via forced oxidation of the intercalated molecules within its interlayers

Yuki Sugiura,* Etsuko Yamada and Masanori Horie

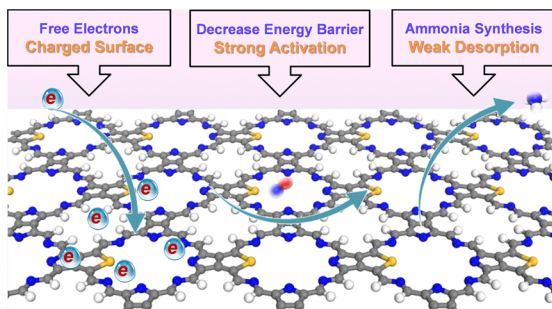
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Tunnel junction sensing of TATP explosive at the single-molecule level

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

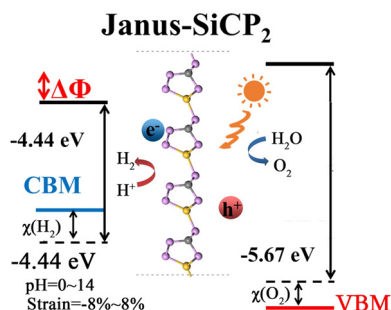
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Theoretical insight into the essential role of charged surface for ammonia synthesis: Si-decorated carbon nitride electrode

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*

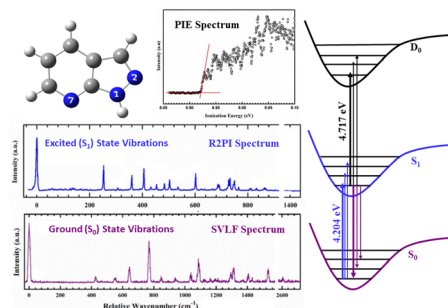


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Laser spectroscopic characterization of supersonic jet cooled 2,7-diazaindole

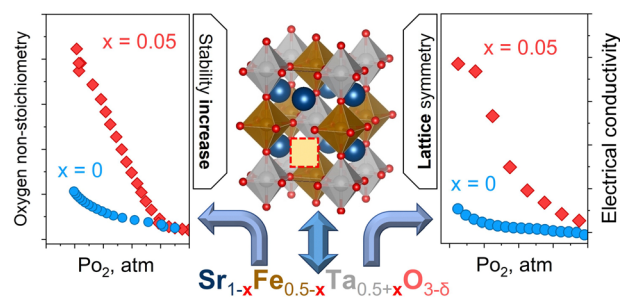
Simran Baweja, Bhavika Kalal and Surajit Maity*



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The influence of strontium deficiency on thermodynamics of defect formation, structural stability and electrical transport of SrFe_{0.5}Ta_{0.5}O_{3-δ}-based solid solutions with an excess tantalum content

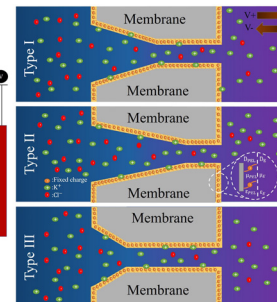
B. V. Politov,* J. C. Waerenborgh, I. R. Shein and O. V. Merkulov



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

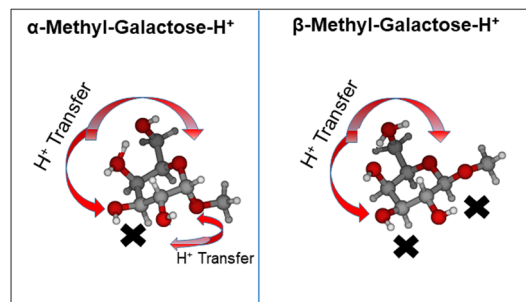
Amirhossein Heydari, Mahdi Khatibi and Seyed Nezameddin Ashrafizadeh*



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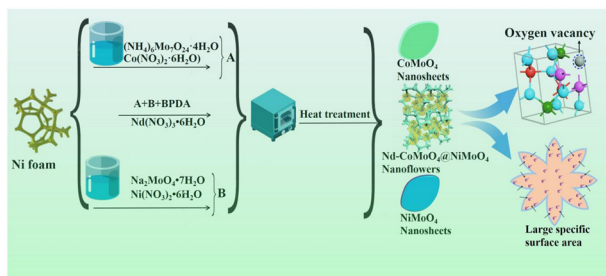
Selective reactivity of glycosyl cation stereoisomers: the role of intramolecular hydrogen bonding

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



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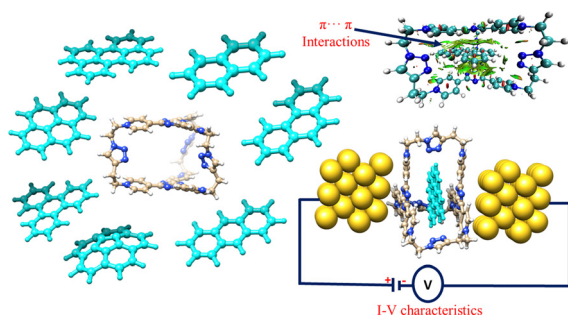
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Coupling of Nd doping and oxygen-rich vacancy in $\text{CoMoO}_4@NiMoO_4$ nanoflowers toward advanced supercapacitors and photocatalytic degradation

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

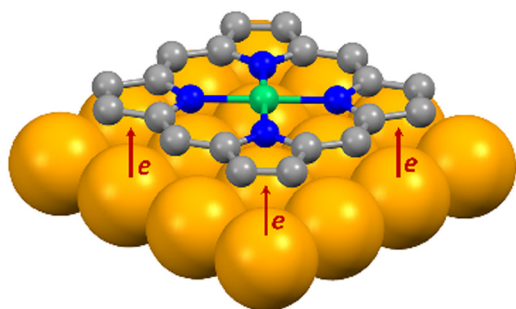
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Exploring $\pi-\pi$ interactions and electron transport in complexes involving a hexacationic host and PAH guest: a promising avenue for molecular devices

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

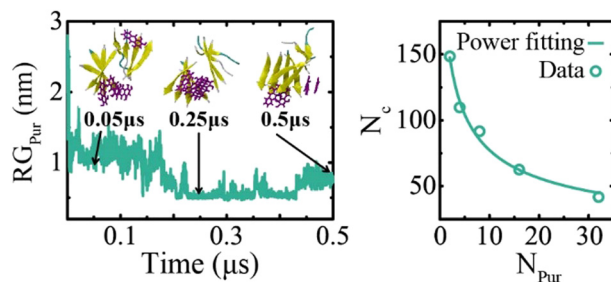
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A local point of view of the $\text{Cu}(100) \rightarrow \text{NiTPP}$ charge transfer at the NiTPP/Cu(100) interface

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

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

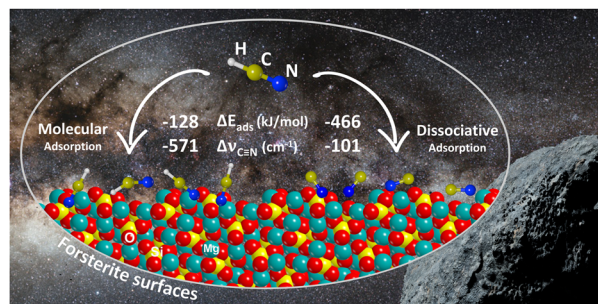
Xiaoxiao Wu, Lili Zhu, Gang Wang, Qingwen Zhang and Zhenyu Qian*



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

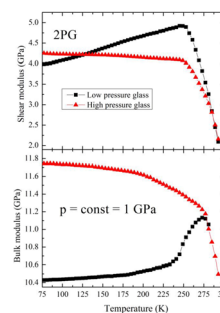
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26813

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

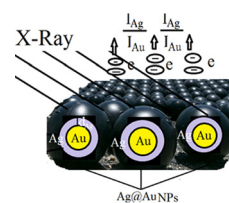
Igor Danilov,* Elena Gromnitskaya and Vadim Brazhkin



26820

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



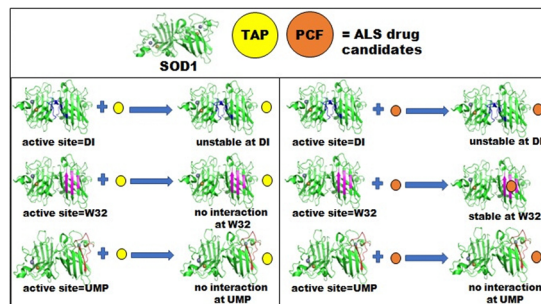
$$d_{Ag} = \lambda_{Au}^{Ag} \cdot \ln \left(1 + \frac{I_{Au}}{I_{Ag}} \frac{\lambda_{Au}^{Au}}{\lambda_{Au}^{Ag} + \lambda_{Au}^{Au}} \frac{I_{Ag}}{I_{Au}} \right)$$

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

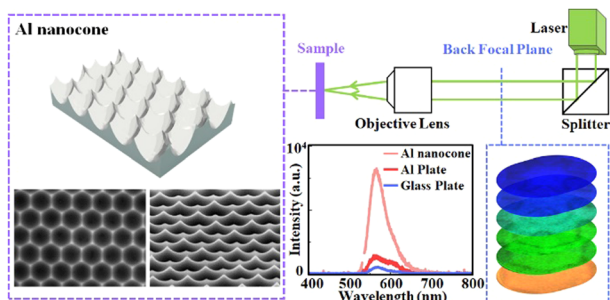
26833

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*



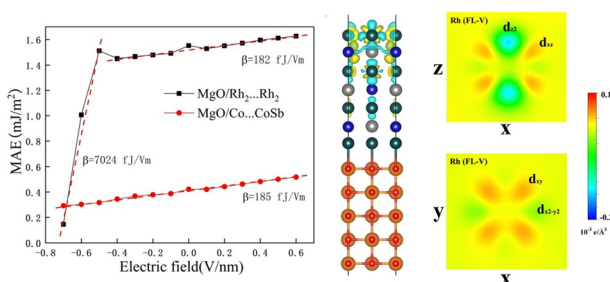
26847



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

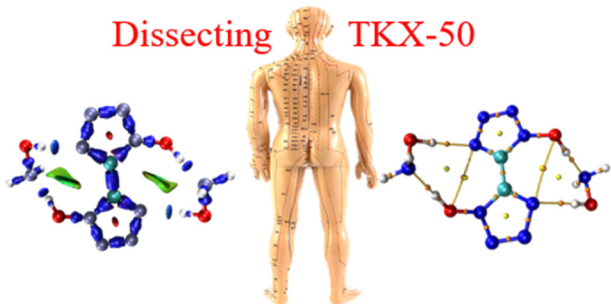


Giant unilateral electric-field control of magnetic anisotropy in MgO/Rh₂CoSb heterojunctions

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

26861

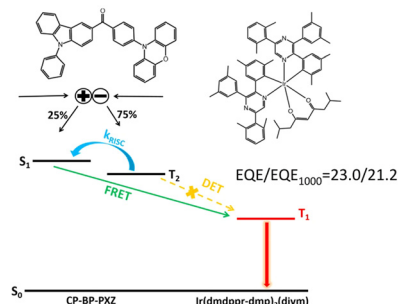
Dissecting TKX-50



Theoretical study on intra-molecule interactions in TKX-50

Chunhai Yang,* Xue Li,* Ning Zhou, Huitong 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

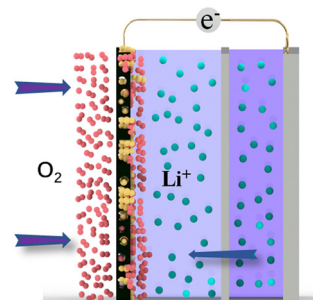
Hanlin Li, Chengwei Lin, Yibing Wu, Xianfeng Qiao, Dezhi Yang, Yanfeng Dai, Qian Sun, Tansir Ahamad, Zhujin Zhao* and Dongge Ma*



26885

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

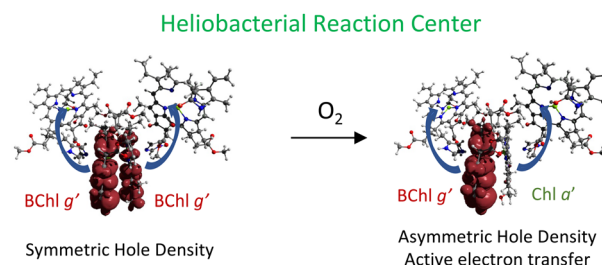
Jie Li, Yuzhi Shi, Junhai Wang, Qianhe Liu, Lihua Luan, Qiang Li, Qinghao Cao, Tianyu Zhang and Hong Sun*



26894

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

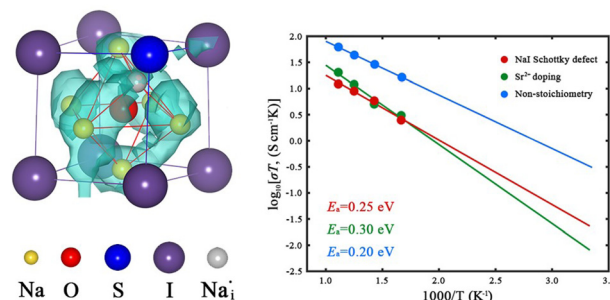
Divya Kaur,* Bryan Ferlez, Patrick Landry, Till Biskup, Stefan Weber, John H. Golbeck,* K. V. Lakshmi* and Art van der Est*



26906

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

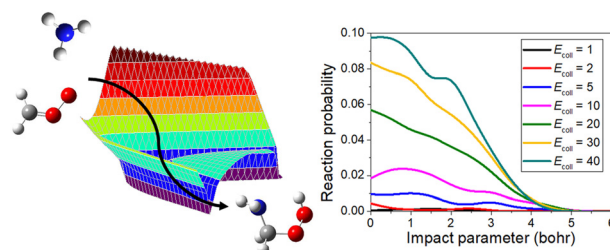
Sen Lian, Congcong Li, Chen Kang, Junfeng Ren and Meina Chen*



26917

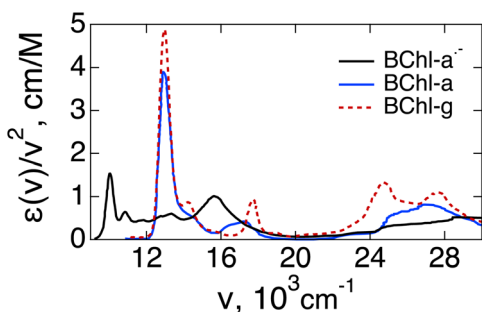
Full-dimensional automated potential energy surface development and detailed dynamics for the CH₂OO + NH₃ reaction

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

