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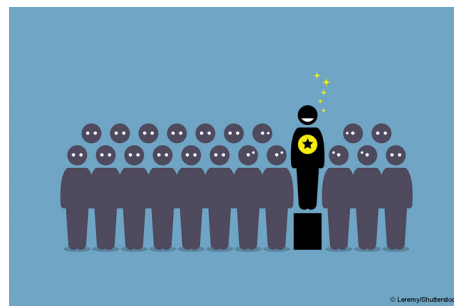
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EDITORIAL

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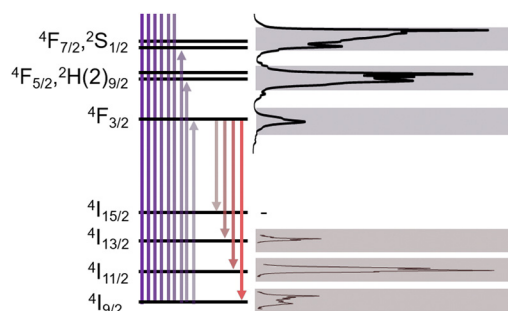


REVIEWS

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Optical spectroscopy as a tool for studying the solution chemistry of neodymium(III)

Patrick R. Nawrocki and Thomas Just Sørensen*



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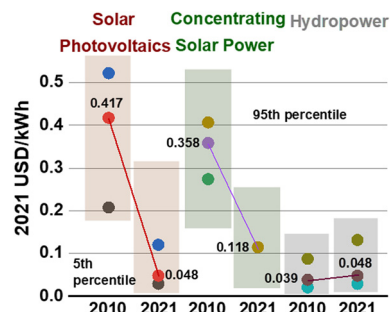


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Prospects of glove-box versus air-processed organic solar cells

Shafket Rasool* and Jin Young Kim*

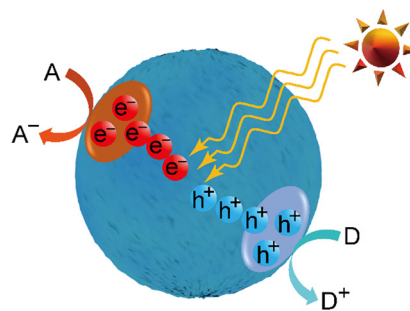


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Schottky-barrier-free plasmonic photocatalysts

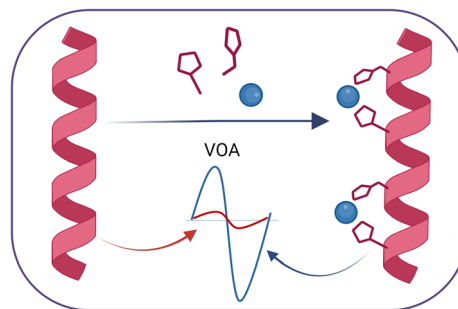
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Chirality induction and amplification in supramolecular systems exhibiting vibrational optical activity

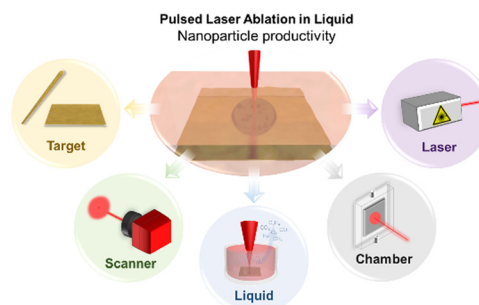
Agnieszka Kaczor



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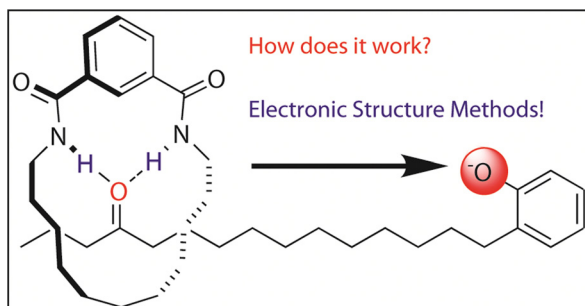
Green nanoparticle synthesis at scale: a perspective on overcoming the limits of pulsed laser ablation in liquids for high-throughput production

Inna Y. Khairani, Gladys Minguez-Vega, Carlos Doñate-Buendía and Bilal Gökce*



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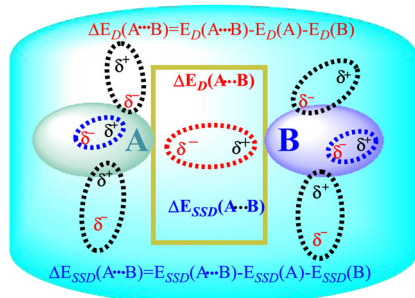


The use of molecular electronic structure methods to investigate mechanically interlocked molecules

Renato Pereira Orenha,* Giovanni Finoto Caramori,*
Renato Luis Tame Parreira* and Alvaro Munoz-Castro

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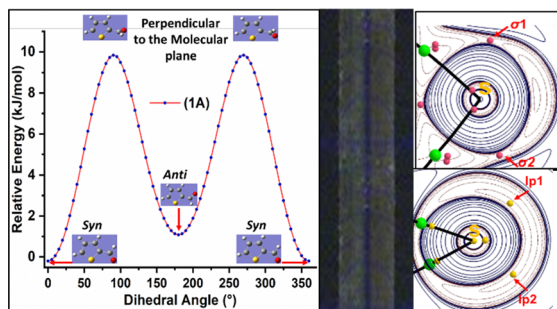
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The treatment of dispersion terms for solution systems

De-Cai Fang,* Si-Cong Liu, Dan-Yang Liu and
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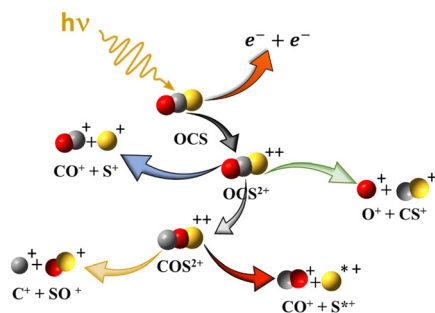


Quantitative evaluation of the electronic features involving "nucleophilic–electrophilic" character in the chalcogen sulfur

Koushik Mandal, Avantika Hasija, Rahul Shukla,*
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Doubly ionized OCS bond rearrangement upon fragmentation – experiment and theory

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Emelie Olsson, Veronica Ideböhn, Richard J. Squibb,
Jérôme Palaudoux, Gunnar Nyman,
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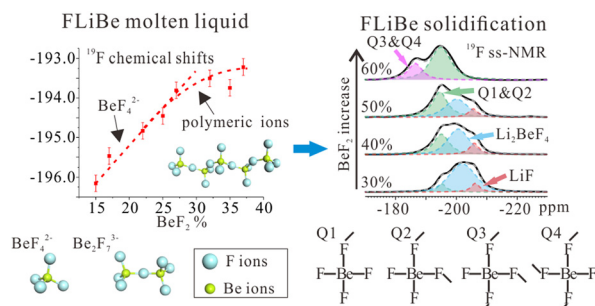


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Probing the local structure of FLiBe melts and solidified salts by *in situ* high-temperature NMR

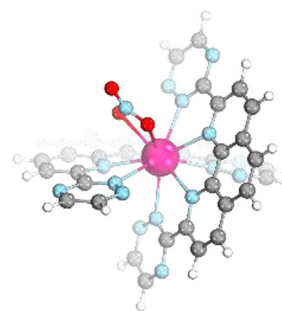
Xiaobin Fu, Yiyang Liu, Hailong Huang, Huiyan Wu, Jianchao Sun, Ling Han, Min Ge, Yuan Qian* and Hongtao Liu*



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The role of covalency in enhancing stability of Eu and Am complexes: a DFT comparison of BTP and BTPPhen

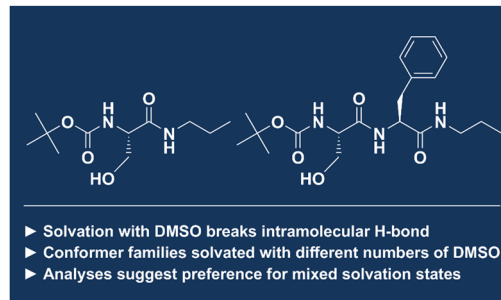
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Solvation of serine-based model peptides and the role of the intramolecular OH...O hydrogen bond in interpreting VCD spectra

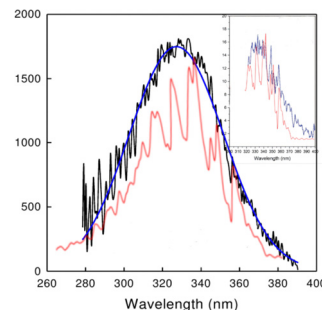
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Photodissociation dynamics and UV absorption spectrum of acetone oxide (CH₃)₂COO

Behnam Nikoobakht* and Horst Köppel



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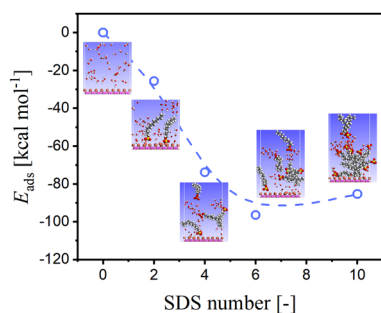
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Charge delocalization and aromaticity of doubly reduced double-walled carbon nanohoos

Rafael Lingas, Nickolas D. Charistos* and Alvaro Muñoz-Castro*

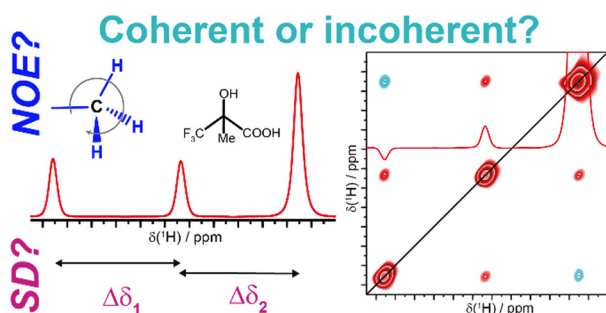
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Refinement of nanoporous copper by dealloying the Al–Cu alloy in NaOH solution containing sodium dodecyl sulfate

Jie Li,* Zhi-Bin Yi, Nuo-Tong Li, Na-Na Yu and Hao-Ran Geng

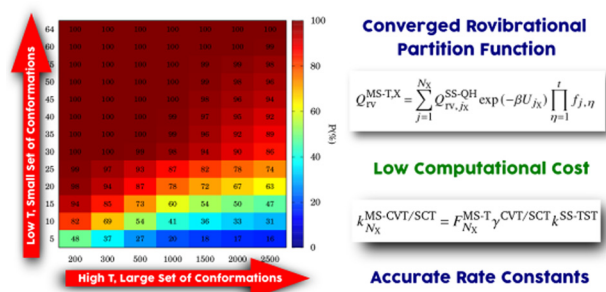
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The effect of methyl group rotation on ^1H – ^1H solid-state NMR spin-diffusion spectra

Ettore Bartalucci, Dominique J. Luder, Nicole Terefenko, Alexander A. Malär, Carsten Bolm, Matthias Ernst* and Thomas Wiegand*

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Multistructural partition function truncation and its effect on the thermal rate constants

Joel Leitão Nascimento, Maiara Oliveira Passos and Tiago Vinicius Alves*

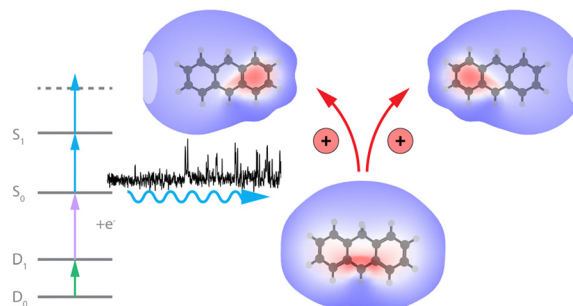


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Intramolecular hole-transfer in protonated anthracene

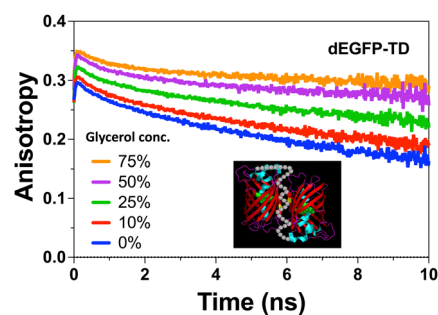
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Ultrafast fluorescence depolarisation in green fluorescence protein tandem dimers as hydrophobic environment sensitive probes

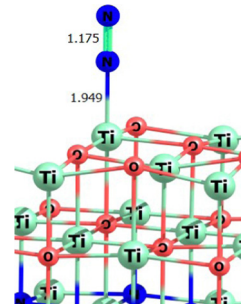
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Stability and activity of titanium oxynitride thin films for the electrocatalytic reduction of nitrogen to ammonia at different pH values

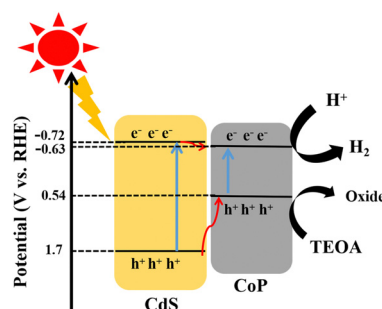
Precious Chukwunenye, Ashwin Ganesan, Mojgan Gharaee, Kabirat Balogun, Qasim Adesope, Stella Chinelo Amagbor, Teresa D. Golden, Francis D'Souza, Thomas R. Cundari and Jeffry A. Kelber*



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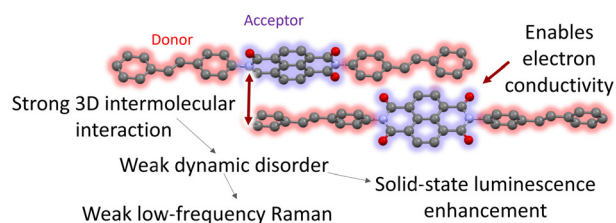
CoP-modified CdS for enhanced stability and photocatalytic hydrogen production under visible light

Zijun Li, Yiqiao Wang, Yongping Luo, Rui Xiao, Hao Ye, Yu Xie,* Yongcun Ma, Yong Chen and Yun Ling



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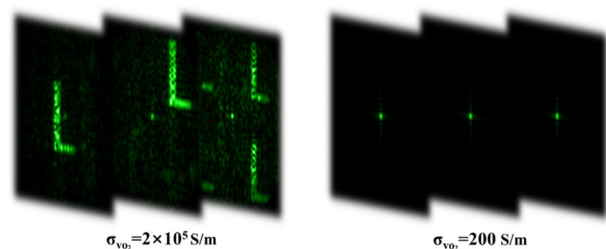
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Structure and properties of naphthalene-diimide *N*-functionalized with stilbene

Andrey Yu. Sosorev,* Igor I. Ponomarev, Dmitry I. Dominskiy, Konstantin A. Lyssenko, Olga D. Parashchuk, Vasily A. Trukhanov, Vladislav G. Konstantinov, Nikita O. Dubinets and Dmitry Yu. Paraschuk

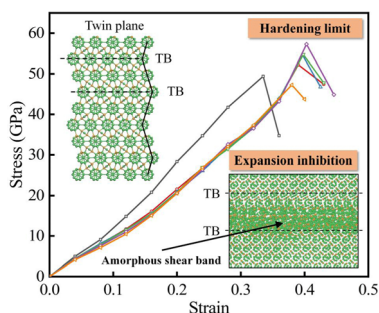
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Terahertz state switching of holograms enabled by vanadium dioxide-based metasurfaces

Chaoxian Tang, Canhui He, Changqing Li and Zhengyong Song*

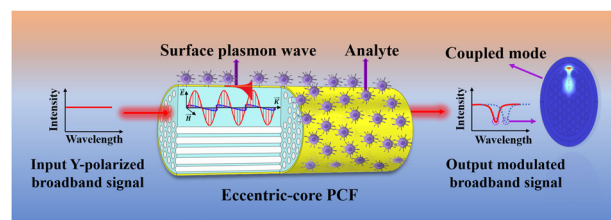
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Superhardness in nanotwinned boron carbide: a molecular dynamics study

Liping Shi, Hongchi Zhang, Xiaoliang Ma, Lin Yang,* Yesheng Zhong* and Xiaodong He*

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Highly sensitive plasmonic sensor based on eccentric-core photonic crystal fibers

Wanlai Zhu, Feng Xu, Zao Yi,* Shubo Cheng, Hua Yang, Xianwen Wu, Gongfa Li, Liangcai Zeng, Zhenfang Yu* and Hailiang Li

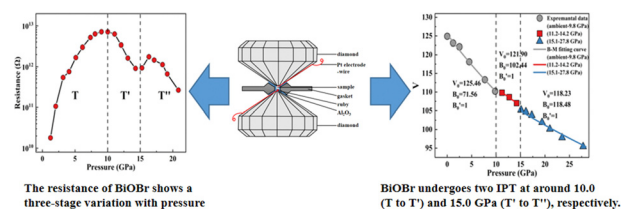


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Study on pressure-induced isostructural phase transition and electrical transport properties of BiOBr

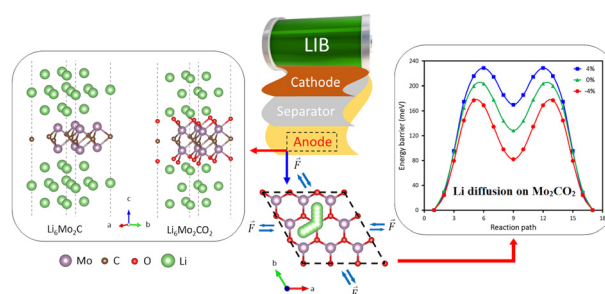
Xiaotong Zhang, Yang Gao,* Zhenfang Xing, Di Peng and Yonghao Han*



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First-principles study of 2H-Mo₂C-based MXenes under biaxial strain as Li-battery anodes

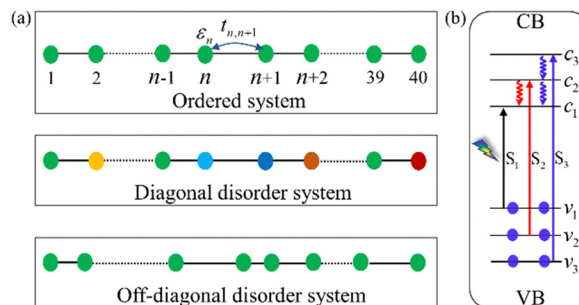
Satchakorn Khammuang, Anucha Pratumma, Aparporn Sakulkalavek, Thanayut Kaewmaraya, Tanveer Hussain and Komsilp Kotmool*



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The effect of the intramolecular disorder on hot exciton dynamics in polymer solar cells

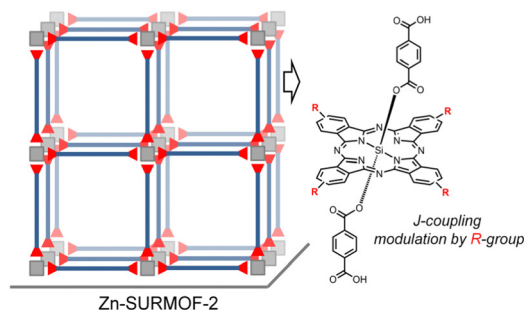
Maomao Zhang, Qiuxia Lu, Xiaojing Liu and Zhong An*



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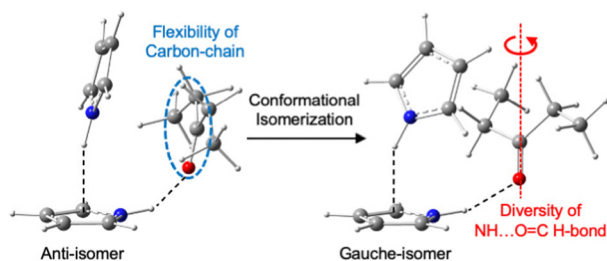
Tunable J-type aggregation of silicon phthalocyanines in a surface-anchored metal–organic framework thin film

Hongye Chen, Luis Martin-Gomis, Zhiyun Xu, Jan C Fischer, Ian A Howard, David Herrero, Víctor Sobrino-Bastán, Ángela Sastre-Santos,* Ritesh Haldar* and Christof Wöll*



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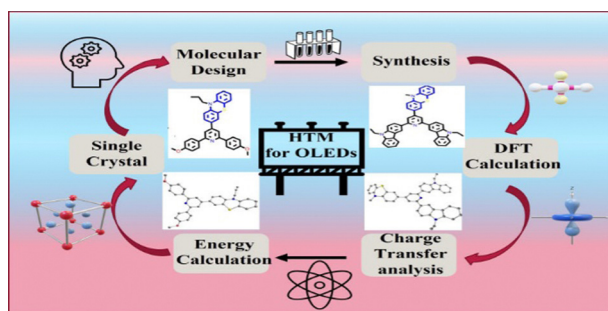
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IR cavity ringdown spectroscopy and density functional theory calculation of pyrrole–diethyl ketone clusters: impacts of carbon-chain flexibility on the diversity of N–H...O=C hydrogen bonds

Yoshiteru Matsumoto* and Kenji Honma

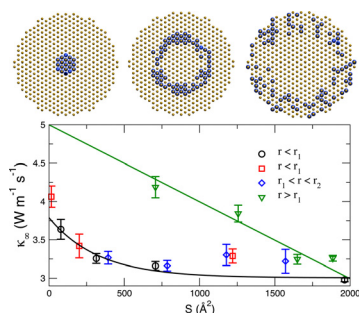
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Rationally heteroarylated pyridines as hole transport materials for OLEDs

Krishan Kumar,* Anirban Karmakar, Feng-Rong Chen, Jwo-Huei Jou, Subrata Ghosh, Subrata Banik* and Sunil Kumar*

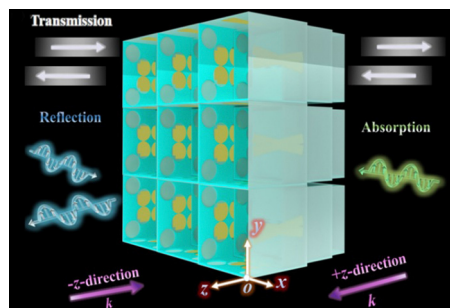
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Effects of vacancies on the thermal conductivity of Si nanowires

Marc Túnica, Paolo Sebastiano Floris, Pol Torres and Riccardo Rurali*

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Broadband plasmon-induced transparency to an anapole mode induced absorption conversion Janus metastructure by a waveguide structure in the terahertz region

Si Ying Li, Zhao Tang, Di Di Zhu and Hai Feng Zhang*

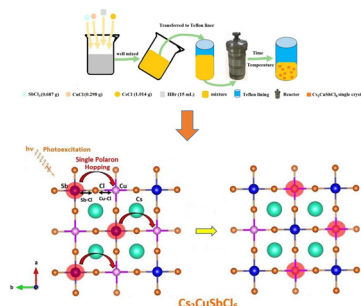


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Understanding the polaron behavior in $\text{Cs}_2\text{CuSbCl}_6$ halide double perovskite

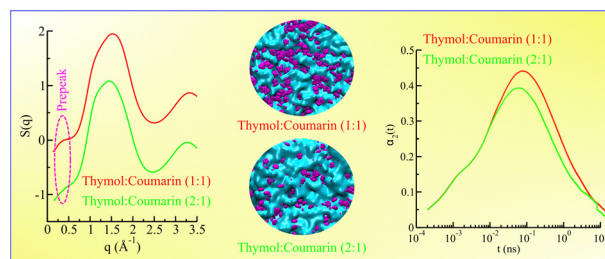
Mohamed Ben Bechir* and Sami Znaidia



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Origin of structural and dynamic heterogeneity in thymol and coumarin-based hydrophobic deep eutectic solvents as revealed by molecular dynamics

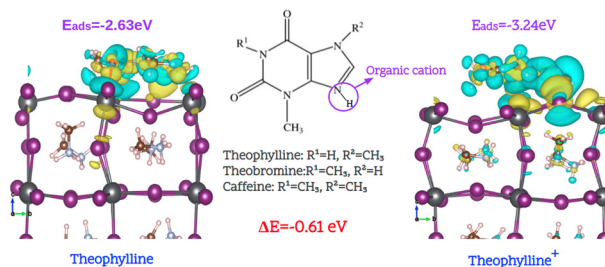
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The role of organic cations as additives in photovoltaic perovskites

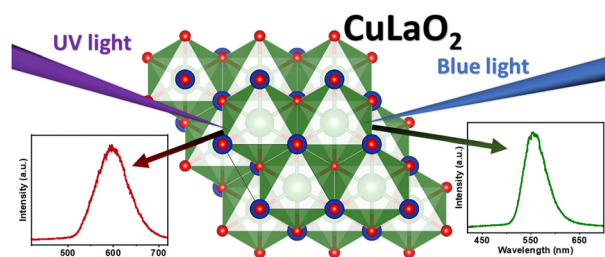
Alejandra T. Cadillo-Martinez, Alejandra Vargas-Calderon, Arián Espinosa-Roa and Andrés M. Garay-Tapia*



19713

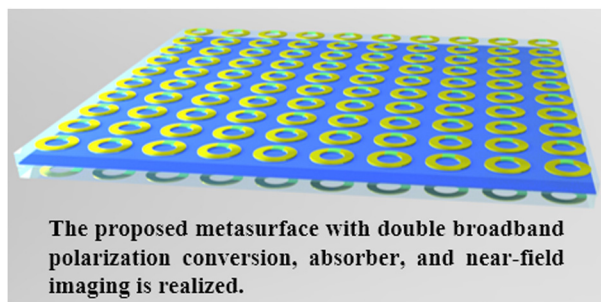
Uncovering the origin of radiationless losses in CuLaO_2 by rationalizing the action of temperature and pressure on luminescence

Mikotaj Kamiński, Sebastian Mahlik,* Anthony Barros and Philippe Boutinaud*



RESEARCH PAPERS

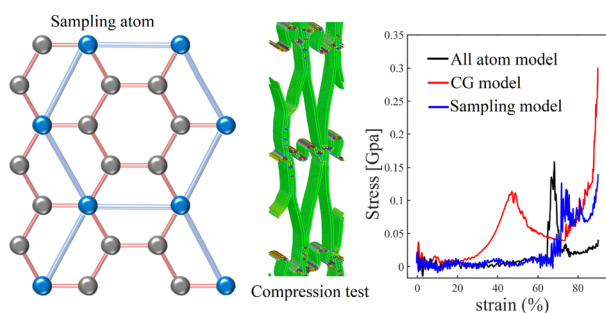
19719



Difunctional terahertz metasurface with switchable polarization conversion and absorption by VO_2 and photosensitive silicon

Guan Wang, Shiyi Zuo, Jia Liu, Xin Zhang, Meichen Li, Shuang Yang, Yang Jia and Yachen Gao*

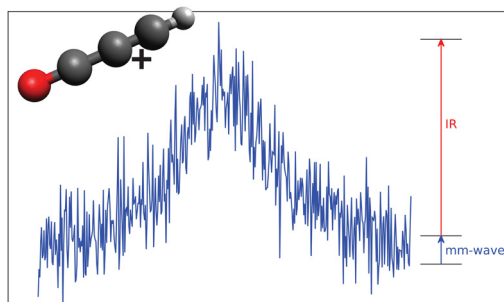
19727



The atom sampling method for mesoscale molecular dynamics and its application to graphene assemblies

Xiong Pan, Hanhui Jin,* Xiaoke Ku and Jianren Fan

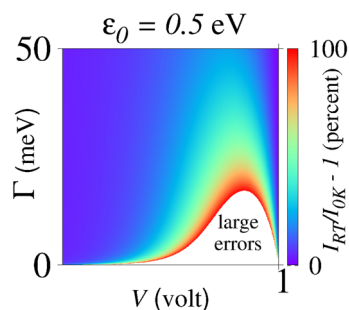
19740



High-resolution ro-vibrational and rotational spectroscopy of HC_3O^+

Oskar Asvany,* Sven Thorwirth, Philipp C. Schmid, Thomas Salomon and Stephan Schlemmer

19750



Can room-temperature data for tunneling molecular junctions be analyzed within a theoretical framework assuming zero temperature?

Ioan Bâldea

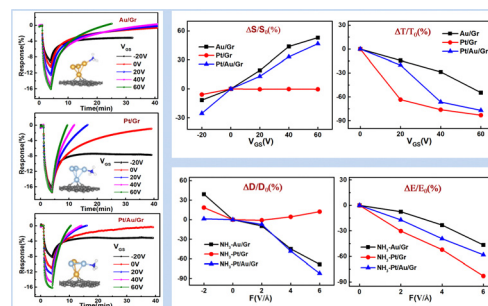


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19764

Unique modulation effects on the performance of graphene-based ammonia sensors via ultrathin bimetallic Au/Pt layers and gate voltages

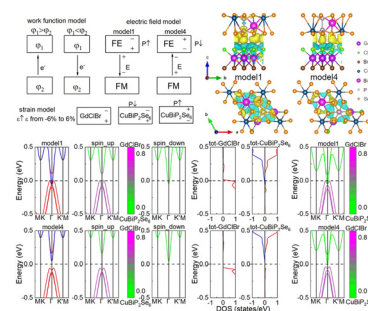
Min Zhao, Yi Tian, Lanqin Yan, Rujun Liu, Peipei Chen,*
Hanfu Wang* and Weiguo Chu*



19773

Spin-splitting and switchable half-metallicity in a van der Waals multiferroic CuBiP₂Se₆/GdClBr heterojunction

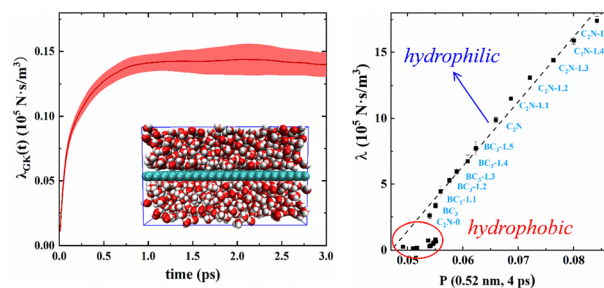
Kai Zhang, Xiaocha Wang* and Wenbo Mi



19788

A numerical model for water hydration on nanosurfaces: from friction to hydrophilicity and hydrophobicity

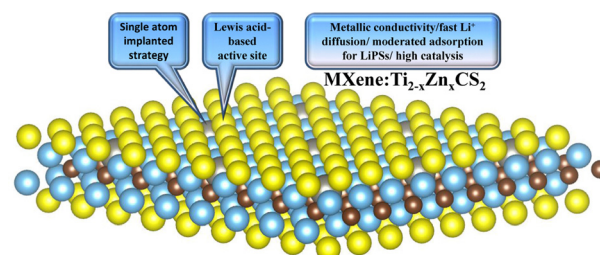
Shuwen Zhang, Zhihao Wang, Chao Ding,
Hongwang Lu,* Yuanyuan Qu, Yong-Qiang Li,
Mingwen Zhao and Weifeng Li*



19795

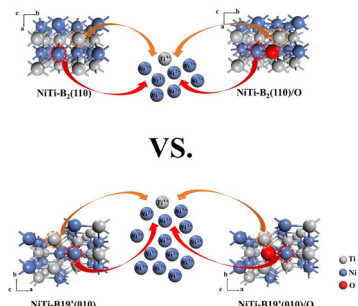
Theoretical identification of the superior anchoring effect and electrochemical performance of Ti₂CS₂ by single atom Zn doping for lithium–sulfur batteries

Mingyang Wang, Jianjun Mao, Yudong Pang, Xilin Zhang,
Haiyan Wang, Zongxian Yang,* Zhansheng Lu* and
Shuting Yang*



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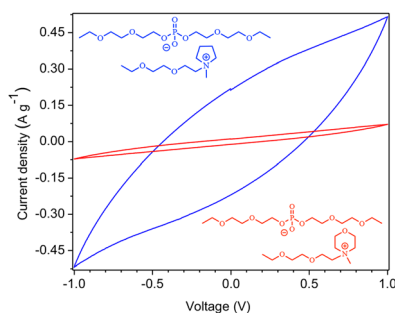
19804



DFT investigation of the dissolution trends of NiTi alloys with the B₂ and B19' phases during the initial oxidation stage

Xiaoting Wang, Dong Xie,* Longjun Wei, Duo You, Mingxi Hou and Yongxiang Leng*

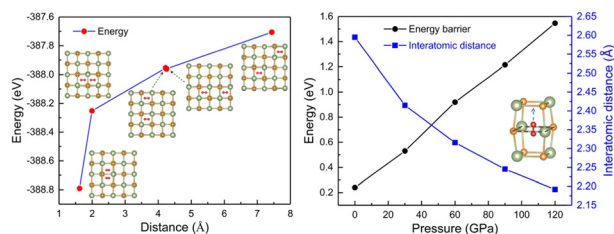
19815



Structurally flexible pyrrolidinium- and morpholinium-based ionic liquid electrolytes

Sourav Bhowmick, Gaurav Tatrari, Andrei Filippov, Patrik Johansson* and Faiz Ullah Shah*

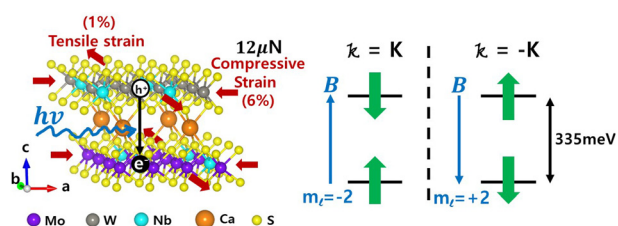
19824



Effects of pressure on hydrogen diffusion behaviors in MgO

Kaishuai Yang, Xixi Tao, Zhi Zeng and Xianlong Wang*

19834



The electronic structure of a strongly bound sandwich MoS₂-WS₂ heterobilayer

Getasew Muluaem Zewdie, Mourad Boujnah, Ju Yeon Kim and Hong Seok Kang*

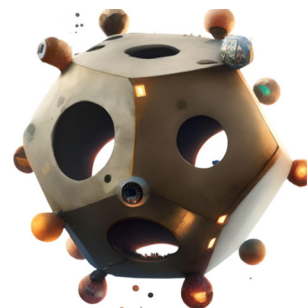


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19845

Cl@Si₂₀X₂₀ cages: evaluation of encapsulation nature, structural rigidity, and ²⁹Si-NMR patterns using relativistic DFT calculations

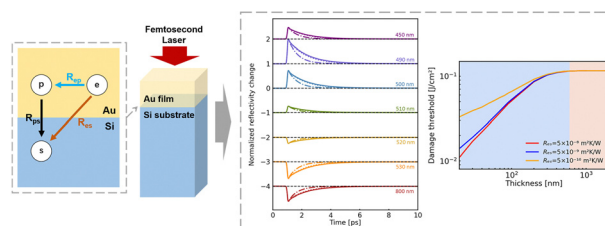
Desmond MacLeod-Carey, Peter L. Rodriguez-Kessler* and Alvaro Muñoz-Castro*



19853

The effect of enhanced heat transfer across metal–nonmetal interfaces subject to femtosecond laser irradiation

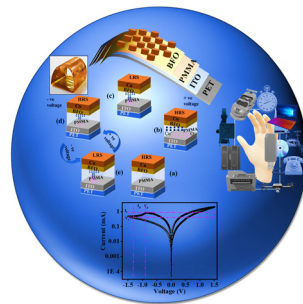
Gen Lin, Lan Jiang and Pengfei Ji*



19868

Low power highly flexible BiFeO₃-based resistive random access memory (RRAM) with the coexistence of negative differential resistance (NDR)

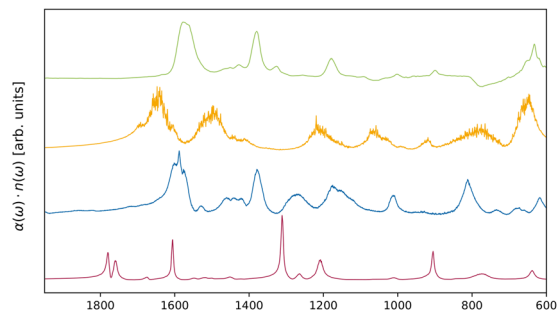
Chandra Prakash, Ankit K. Yadav and Ambesh Dixit*



19882

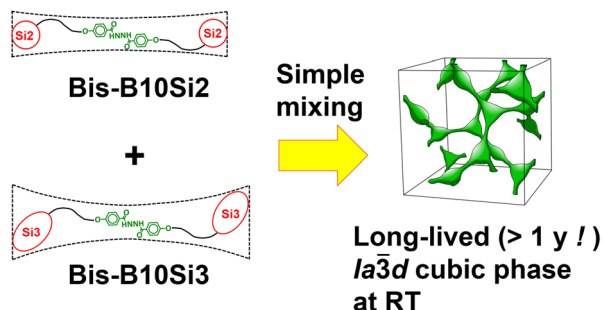
Force field refinement for reproducing experimental infrared spectra of ionic liquids

András Szabadi, Aleksandar Doknic, Jonathan Netsch, Ádám Márk Pálvögyi, Othmar Steinhauser and Christian Schröder*



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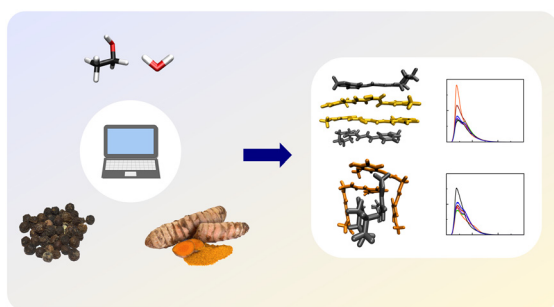
19891



Room-temperature *la* $\bar{3}$ *d* phase obtained for the binary mixture containing different sizes of siloxanyl terminals

Yuki Kawase, Shoichi Kutsumizu,* Taro Udagawa, Yohei Miwa, Yasuhisa Yamamura and Kazuya Saito

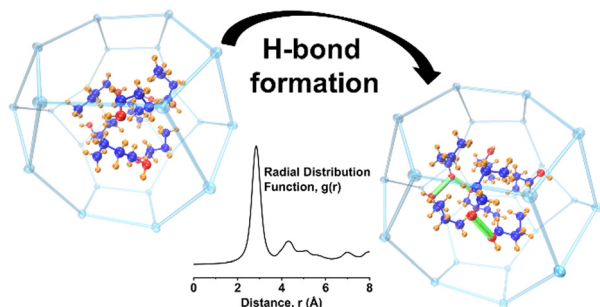
19899



Aggregation patterns of curcumin and piperine mixtures in different polar media

J. R. C. Santos, P. E. Abreu and J. M. C. Marques*

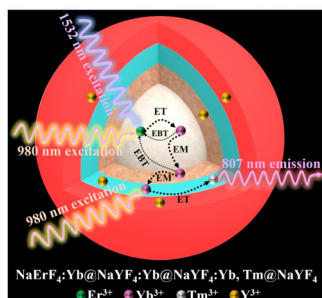
19911



An investigation into the adsorption mechanism of *n*-butanol by ZIF-8: a combined experimental and *ab initio* molecular dynamics approach

Samuel P. Wallbridge, Stuart Archer, Mark R. J. Elsegood, Jonathan L. Wagner, Jamieson K. Christie and Sandra E. Dann*

19923



High-intensity first near-infrared emission through energy migration in multilayered upconversion nanoparticles

Xuegang Zheng, Ying Chen, Meijuan Liu, Shusheng Pan, Zhiyu Liu, Dekang Xu and Hao Lin*

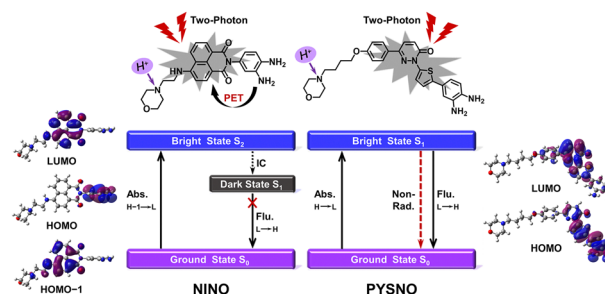


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19932

Theoretical characterization of two-photon fluorescent probes for nitric oxide detection: sensing mechanism, photophysical properties and protonation effects

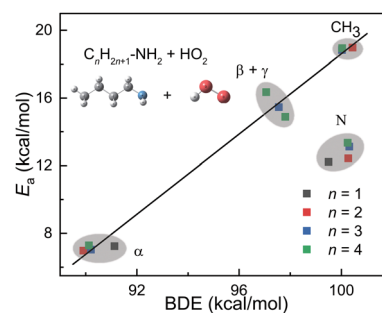
Yawen Jiao, Xiaoxu Dong, Xin Ran, Qiyun Deng, Haibin Xiao, Zhiming Wang* and Tian Zhang*



19943

Theoretical study of hydrogen abstraction by HO₂ radicals from primary straight chain amines C_nH_{2n+1}-NH₂ (n = 1–4)

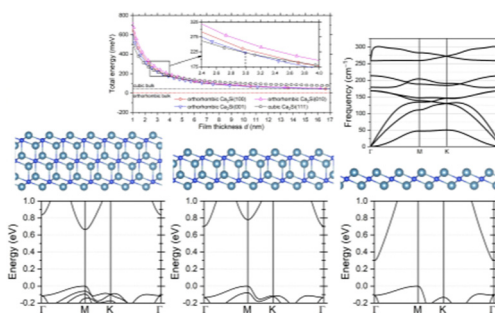
Yi Bao, Xiaoyi Liu, Zezhou He and Jinchun Shi*



19952

Interplay between structural changes, surface states and quantum confinement effects in semiconducting Mg₂Si and Ca₂Si thin films

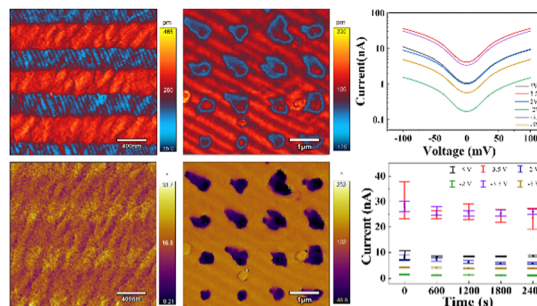
A. Yu. Alekseev, D. B. Migas,* A. B. Filonov, N. G. Galkin and N. V. Skorodumova



19963

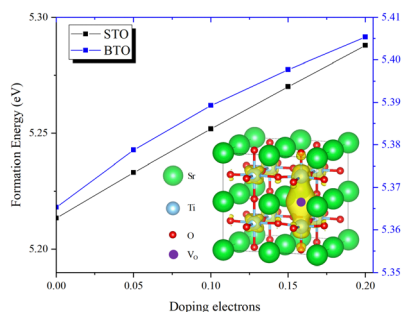
An electric-field-driven ferroelectric nanodomain structure and its multilevel data storage application

Pengfei Hou,* Zixian Lian and Cheng Chen



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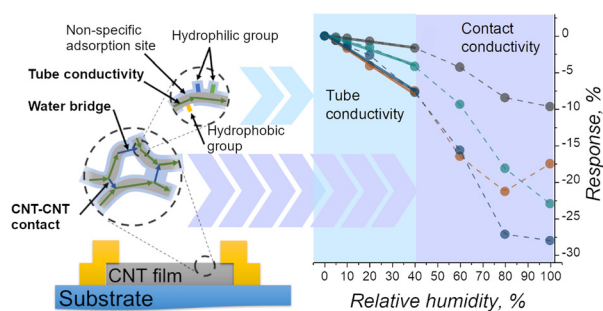
19970



Stability of oxygen vacancies at metal/oxide interfaces

Xingwen Zheng, Ying Yang, Changfeng Fang* and Xiaohui Liu*

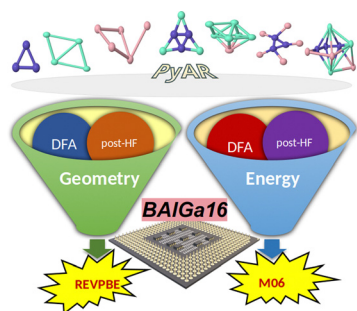
19976



Tuning humidity sensing properties via grafting fluorine and nitrogen-containing species on single-walled carbon nanotubes

Vitalii I. Sysoev,* Olga A. Gurova, Yuliya V. Fedoseeva, Artem V. Gusel'nikov, Anna A. Makarova, Alexander V. Okotrub and Lyubov G. Bulusheva

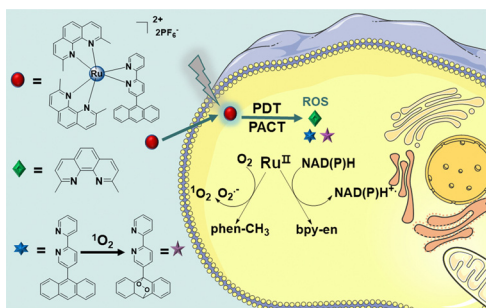
19986



Nanoclusters and nanoalloys of group 13 elements (B, Al, and Ga): benchmarking of methods and analysis of their structures and energies

Maya Khatun, Pratik Sarkar, Sunanda Panda, Lazumla T. Sherpa and Anakuthil Anoop*

20001



Novel Ru(II) complexes with multiple anticancer photoreactivity: ligand exchange, photoredox catalysis, reactive oxygen generation and endoperoxide formation

Anyi Dao, Haorui Wu, Siqi Wei and Huaiyi Huang*

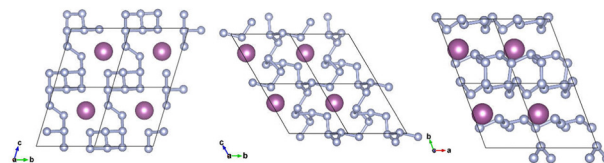


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20009

Prediction of metastable phase of the Sc–N system in the N-rich region under high pressure

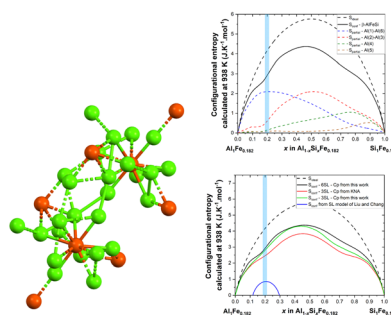
Shifeng Niu, Yuanyuan Liu, Zhenxing Yang, Shijie Liu* and Zhen Yao*



20015

Investigating the Al/Si mixed site occupancy in the β -AlFeSi phase

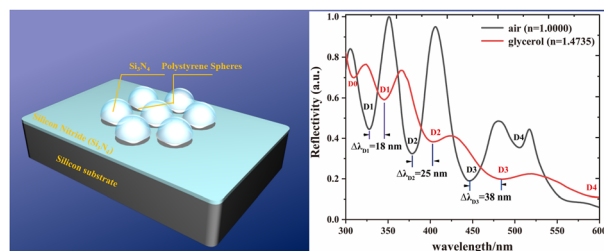
Paul Lafaye,* Minh Duc Vo, Javier Jofre and Jean-Philippe Harvey



20026

Multi-band optical resonance of all-dielectric metasurfaces toward high-performance ultraviolet sensing

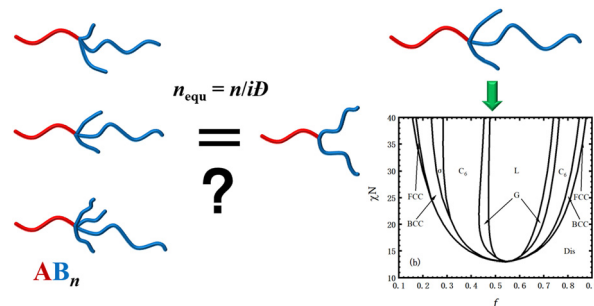
Jie Zheng,* Cheng Zhang, Hong Li, Xianchao Liu, Yijia Huang, Jianqi Zhu, Zhilin Yang and Ling Li*



20032

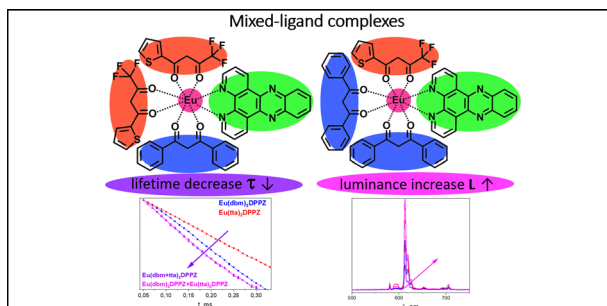
The impact of intramolecular polydispersity on the self-assembly of AB_n miktoarm star copolymers

Jiahao Shi, Xianbo Huang* and Weihua Li*



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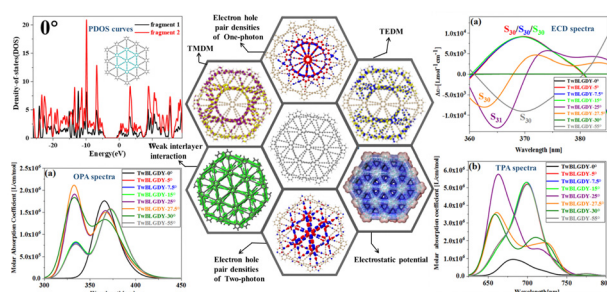
20042



The increase of europium-based OLED luminance through reducing the excited state lifetime by mixed-ligand complex formation

Makarii I. Kozlov,* Andrey A. Vashchenko, Alexander A. Pavlov, Alexander S. Goloveshkin, Egor V. Latipov, Natalia P. Kuzmina and Valentina V. Utochnikova*

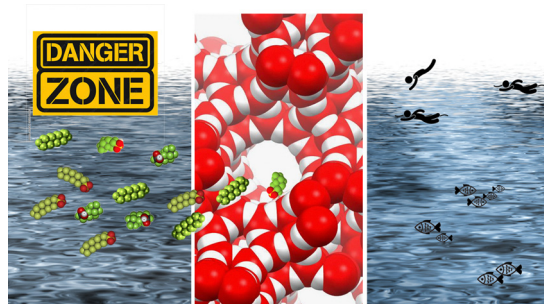
20049



Physical mechanism on the linear spectrum and nonlinear spectrum in a twist bilayer graphdiyne nanodisk

Xinwen Gai, Hao Sheng* and Jingang Wang*

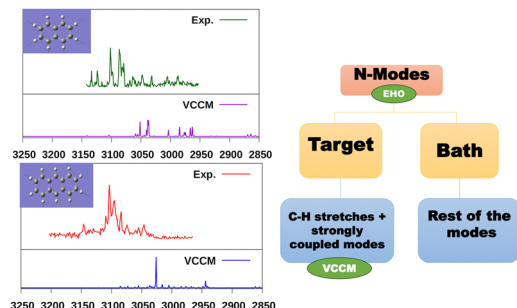
20066



High temperature behaviour of Ag-exchanged Y zeolites used for PFAS sequestration from water

Maura Mancinelli, Annalisa Martucci,* Gian Marco Salani, Gianluca Bianchini,* Lara Gigli, Jasper Rikkert Plaisier and Francesco Colombo

20076



An approximation to the vibrational coupled-cluster method for CH-stretching of large molecules: application to naphthalene and anthracene

Nivedhitha Palanisamy and Subrata Banik*

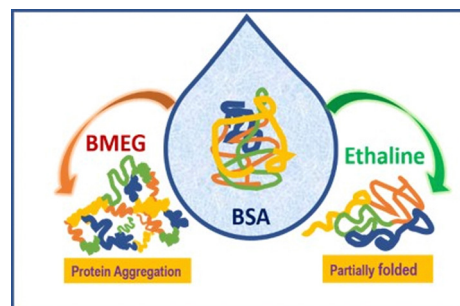


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20093

Assessing the impact of choline chloride and benzyltrimethylammonium chloride-based deep eutectic solvents on the structure and conformational dynamics of bovine serum albumin: a combined steady-state, time-resolved fluorescence and fluorescence correlation spectroscopic study

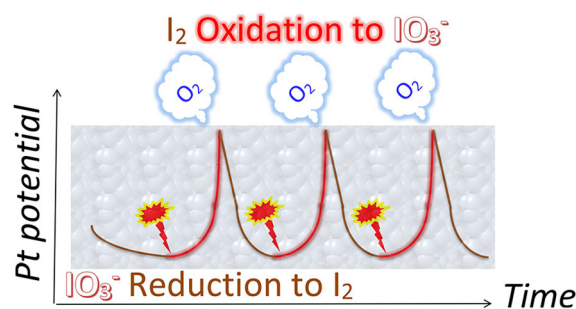
Sahadev Barik, Amita Mahapatra, Naupada Preeyanka and Moloy Sarkar*



20109

Changing the paradigm in modelling the Bray–Liebhafsky oscillatory chemical reaction

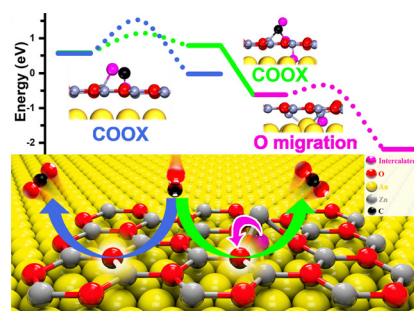
Dragomir Stanisavljev, Annette Fiona Taylor and Itana Nuša Bubanja*



20121

Activating lattice oxygen of single-layer ZnO for the catalytic oxidation reaction

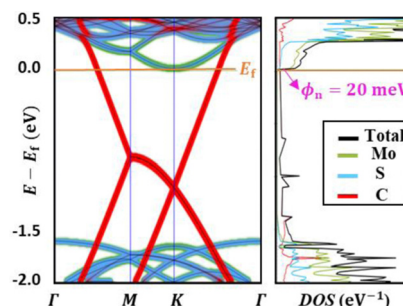
Changping Liu, Le Lin, Hao Wu, Yijing Liu, Rentao Mu* and Qiang Fu*



20128

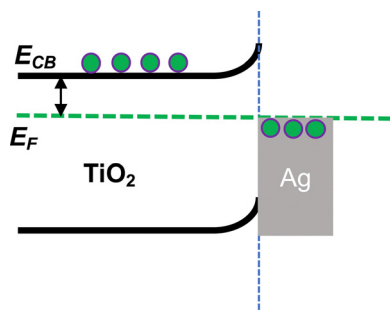
Transition from Schottky to ohmic contacts in the C₃₁ and MoS₂ van der Waals heterostructure

Lijun Xu, Guohui Zhan, Kun Luo, Fei Lu, Shengli Zhang* and Zhenhua Wu*



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20134



Fermi-level shift, electron separation, and plasmon resonance change in Ag nanoparticle-decorated TiO₂ under UV light illumination

Wenhao Zhao, Liping Wen, Ivan P. Parkin, Xiujuan Zhao and Baoshun Liu*

CORRECTION

20145

Correction: Limitations of non-polarizable force fields in describing anion binding poses in non-polar synthetic hosts

David Seiferth, Stephen J. Tucker and Philip C. Biggin*

