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ISSN 1463–9076 CODEN PPCPFQ 25(40) 26933–27894 (2023)



### Cover

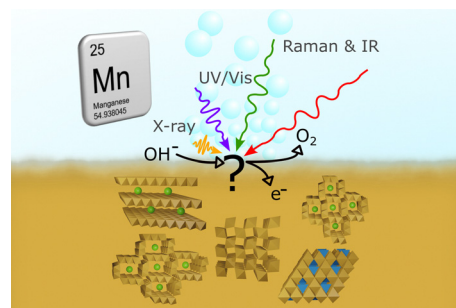
See Andreas Erbe, Marc Frederic Tesch, Martin Rabe *et al.*, pp. 26958–26971. Image reproduced by permission of Tianyi You, Martin Rabe, Andreas Erbe and Marc Frederic Tesch from *Phys. Chem. Chem. Phys.*, 2023, 25, 26958.

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### Operando studies of Mn oxide based electrocatalysts for the oxygen evolution reaction

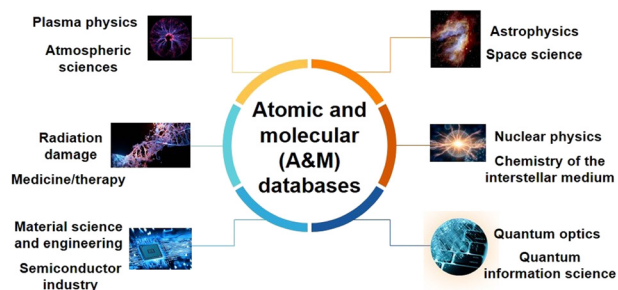
Andreas Erbe,\* Marc Frederic Tesch,\* Olaf Rüdiger, Bernhard Kaiser, Serena DeBeer and Martin Rabe\*



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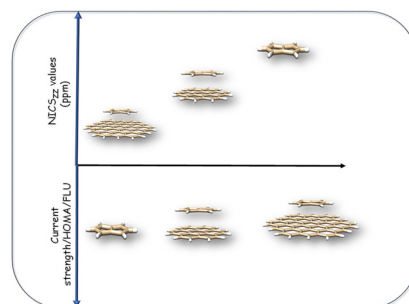


## COMMUNICATION

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## Exploring the influence of graphene on antiaromaticity of pentalene

Keerthy P. Sudhakaran, Alfy Benny, Athira T. John and Mahesh Hariharan\*

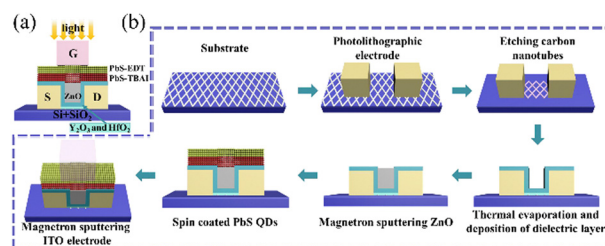


## RESEARCH PAPERS

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## A near-infrared photodetector based on carbon nanotube transistors exhibits ultra-low dark current through field-modulated charge carrier transport

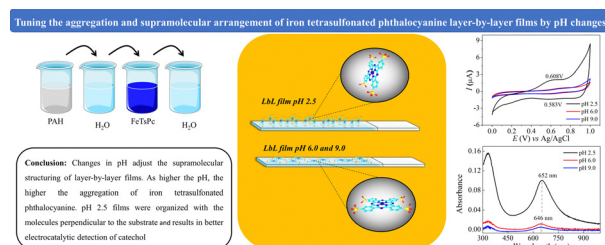
Sheng Wang, Wuhua Huang, Junlong Tian,\* Jie Peng and Juexian Cao\*



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## Controlling supramolecular structures in iron tetrasulfonated phthalocyanine films through pH variation: implications for thin-film device performance

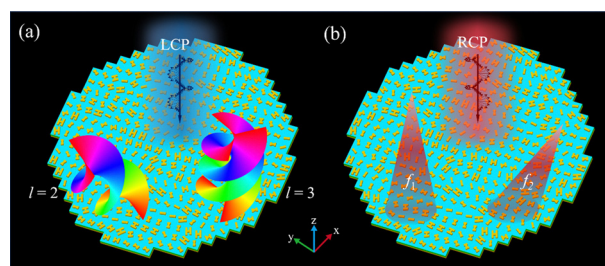
Henry S. Kavazoi,\* Cibely S. Martin, Mateus D. Maximino, Matheus S. Pereira, Maria L. Rodriguez-Méndez and Priscila Alessio\*



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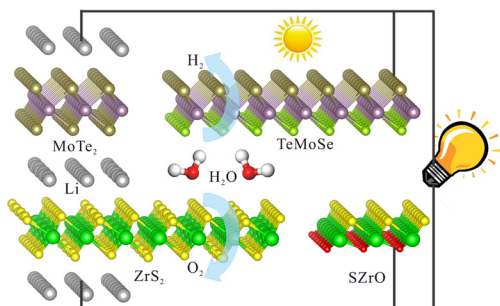
## Optical reflective metasurfaces enable spin-decoupled OAM and focusing

Jinhao Xin, Zhiqiang Du, Zekai Zhou and Zhengyong Song\*



## RESEARCH PAPERS

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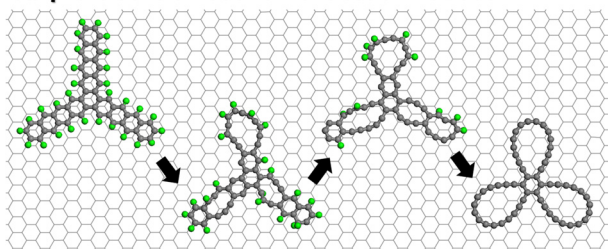


### Substitutional doping of MoTe<sub>2</sub>/ZrS<sub>2</sub> heterostructures for sustainable energy related applications

Xiao-Hua Li, Bao-Ji Wang,\* Xue-Feng Yang, Wei-Yang Yu and San-Huang Ke\*

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### Starphene transformation under electron irradiation in HRTEM

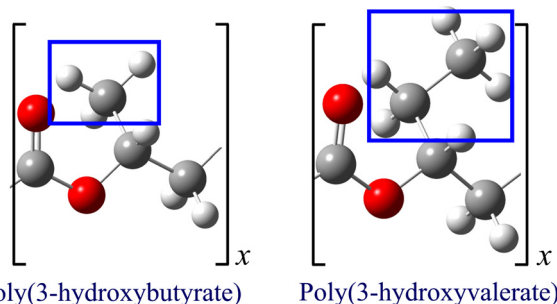


Molecular dynamics simulation by CompuTEM algorithm

### Formation of carbon propeller-like molecules from starphenes under electron irradiation

Nikita A. Matsokin, Alexander S. Sinitsa,\* Yulia G. Polynskaya, Irina V. Lebedeva, Andrey A. Knizhnik and Andrey M. Popov

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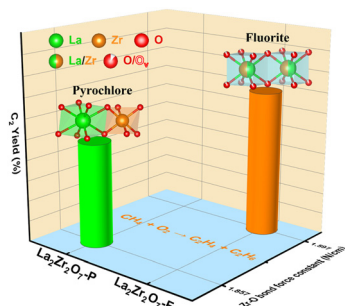
Poly(3-hydroxybutyrate)

Poly(3-hydroxyvalerate)

### Conformational characteristics of poly(3-hydroxyvalerate) (P3HV) and structure–property relationships of P3HV and poly(3-hydroxybutyrate)

Yota Watabe, Shunsuke Shimomura, Koyo Ono and Yuji Sasanuma\*

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### Preparation of La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> composite oxides with fluorite/pyrochlore phases by excluding element influences for catalyzing oxidative coupling of methane

Junwei Xu, Xusheng Zhong, Rumeng Ouyang, Ying Gong, Yameng Liu, Xianglan Xu, Xiuzhong Fang and Xiang Wang\*

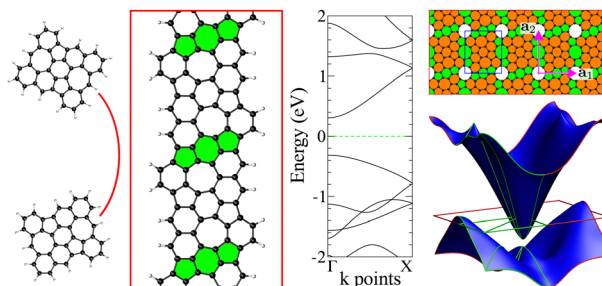


## RESEARCH PAPERS

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### Electronic properties and carrier mobilities of nanocarbons formed by non-benzoidal building blocks

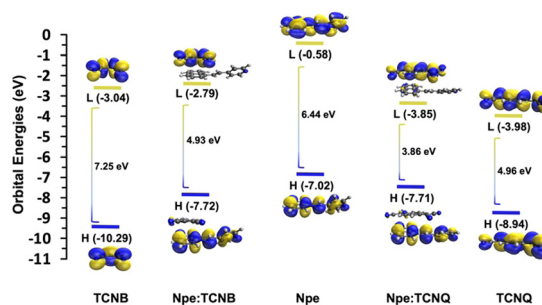
João Alberto Santos Porto, David Joseph Pereira Beserra, Fabrício Morais de Vasconcelos, Paloma Vieira Silva and Eduardo Costa Girão\*



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### Comparing the structures and photophysical properties of two charge transfer co-crystals

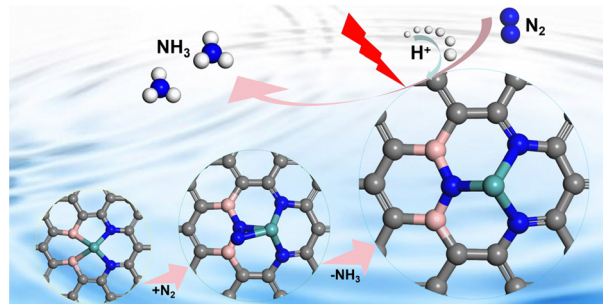
Ali Abou Taka, Joseph E. Reynolds III, Neil C. Cole-Filipiak, Mohana Shivanna, Christine J. Yu, Patrick Feng, Mark D. Allendorf, Krupa Ramasesha, Vitalie Stavila and Laura M. McCaslin\*



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### Molecular nitrogen induced structural evolution of single transition metal atoms supported by B/N co-doped graphene for enhanced nitrogen electroreduction performance

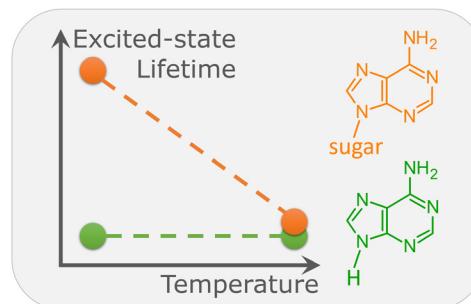
Zhiqiang Bai, Jian Wang,\* Xiaomeng Peng, Yufang Liu\* and Wenhua Zhang\*



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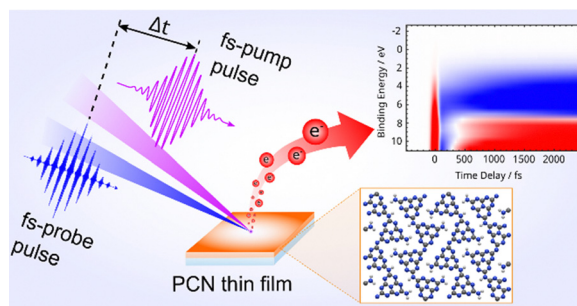
### Temperature effects on the internal conversion of excited adenine and adenosine

Ritam Mansour, Josene M. Toldo,\* Saikat Mukherjee, Max Pinheiro Jr and Mario Barbatti\*



## RESEARCH PAPERS

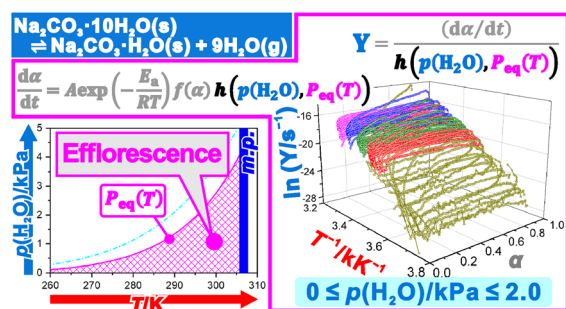
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### Ultrafast dynamics in polymeric carbon nitride thin films probed by time-resolved EUV photoemission and UV-Vis transient absorption spectroscopy

Nataliia Kuzkova, Igor Yu. Kiyan, Iain Wilkinson and Christoph Merschjann\*

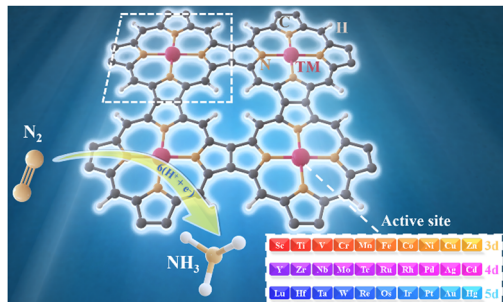
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### Efflorescence kinetics of sodium carbonate decahydrate: a universal description as a function of temperature, degree of reaction, and water vapor pressure

Mito Hotta, Yuto Zushi, Shun Iwasaki, Shunsuke Fukunaga and Nobuyoshi Koga\*

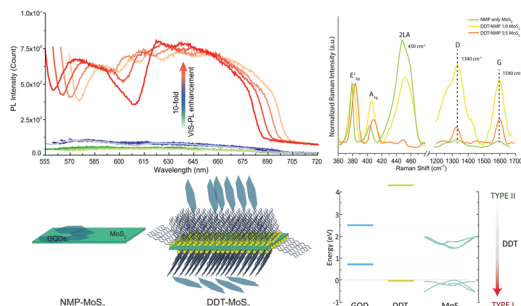
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### Electrochemical ammonia synthesis under ambient conditions using TM-embedded porphine-fused sheets as single-atom catalysts

Ying Yao, Sheng-Yao Lv, Guoliang Li\* and Li-Ming Yang\*

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### Experimental and theoretical investigation of synthesis and properties of dodecanethiol-functionalized MoS<sub>2</sub>

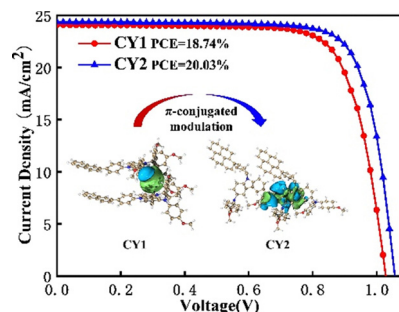
Tuna A. Duran, Denis Šabani, Milorad V. Milošević and Hasan Sahin\*



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### Theoretical calculations and experimental investigation toward the $\pi$ -conjugated modulation in arylamine derivative-based hole transporting materials for perovskite solar cells

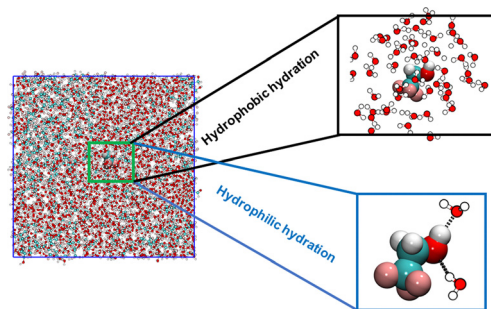
Chengyu Wu, Ruiqin Wang, Jiayi Qi, Xin Chen, Fei Wu\* and Xiaorui Liu\*



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### Impact of hydrophobicity on local solvation structures and its connection with the global solubilization thermodynamics of amphiphilic molecules

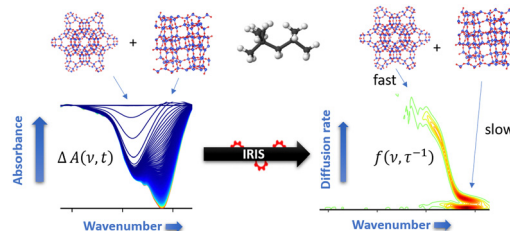
Bibhab Bandhu Majumdar, Partha Pyne, Rajib Kumar Mitra\* and Debasish Das Mahanta\*



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### Study of the diffusion properties of zeolite mixtures by combined gravimetric analysis, IR spectroscopy and inversion methods (IRIS)

Abdelhafid Ait Blal,\* Dusan Stosic, Philippe Bazin, Alexandre Vimont and Arnaud Travert\*

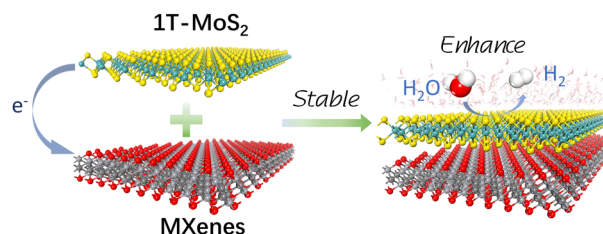


$$f(v, \tau^{-1}) = \operatorname{argmin}_f \left( \left\| \Delta A(v, t) - \int_0^\infty f(v, \tau^{-1}) K(t, \tau^{-1}) d\tau^{-1} \right\|^2 + \lambda S[f] \right)$$

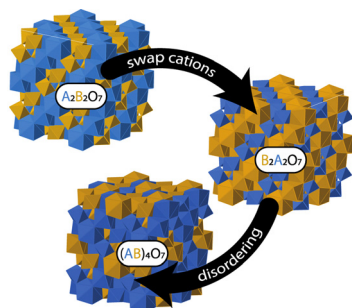
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### A general strategy to stabilize 1T-MoS<sub>2</sub> using MXene heterostructures and unlock its hydrogen evolution reaction capabilities

Yumiao Tian, Xiaochun Liu, Pengfei Hou, Yu Xie, Fei Du, Gang Chen, Aleksandra Vojvodic and Xing Meng\*



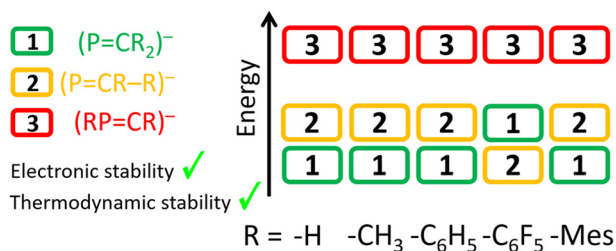
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## How inversion relates to disordering tendencies in complex oxides

Vancho Kocovski, Ghanshyam Pilania and Blas P. Uberuaga\*

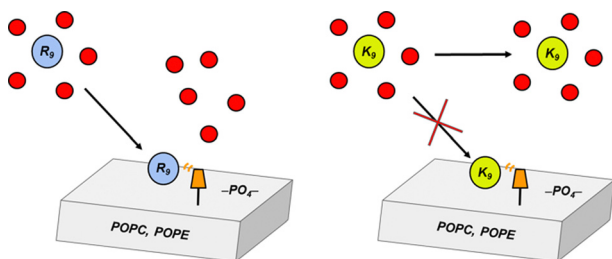
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## An *ab initio* study on the stability of isolated phosphalkene synthons

Adrianna Cyraniak, Sylwia Freza and Piotr Skurski\*

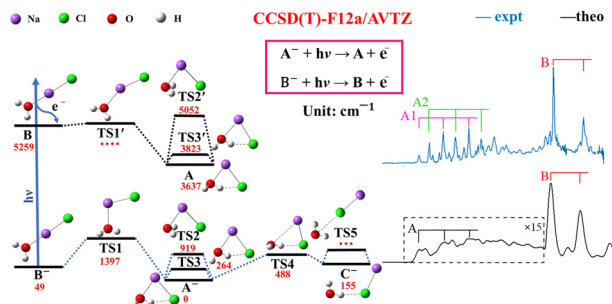
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## Why do polyarginines adsorb at neutral phospholipid bilayers and polylysines do not? An insight from density functional theory calculations and molecular dynamics simulations

Carmelo Tempra, Zlatko Brkljača and Mario Vazdar\*

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## Benchmark computational investigations for the basic model of the salt–water complex: NaCl(H<sub>2</sub>O) and its anion NaCl(H<sub>2</sub>O)<sup>−</sup>

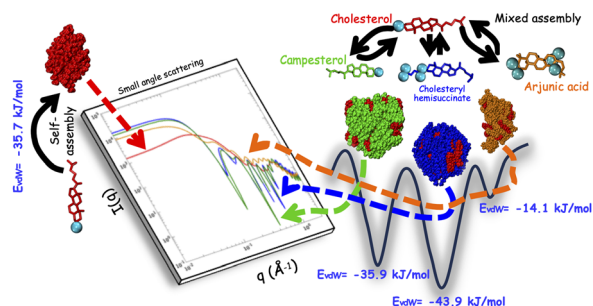
Qi Zhang and Jun Li\*



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## Robustness of heteroaggregates involving hydrophobic cholesterol and its mimetics

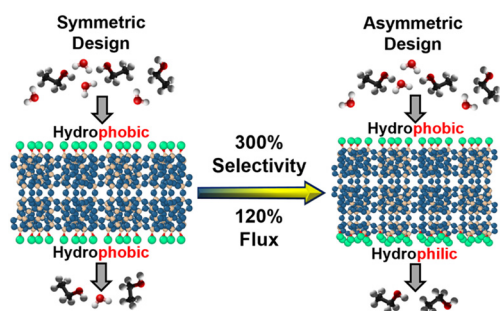
Rituparna Hazra and Durba Roy\*



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## Asymmetric nanoporous membranes for ethanol/water pervaporation separation and their design

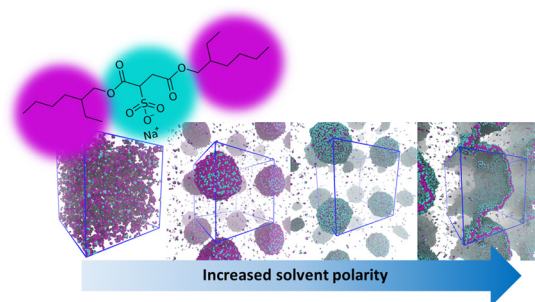
Ting-Yuan Wang, Changlong Zou\* and Li-Chiang Lin\*



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## Diocetyl sodium sulfosuccinate surfactant self-assembly dependency of solvent hydrophilicity: a modelling study

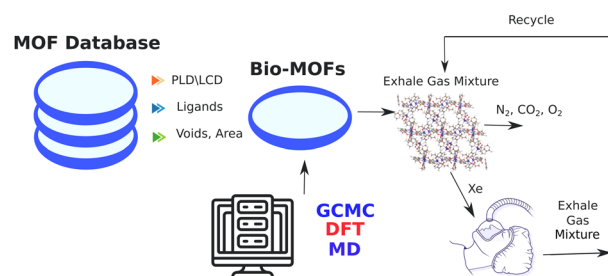
Maisa Vuorte, Apo Lokka, Alberto Scacchi and Maria Sammalkorpi\*



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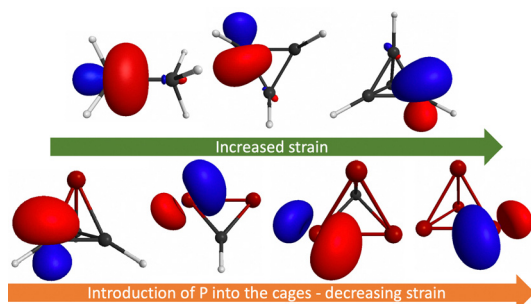
## Noncovalent chemistry of xenon opens the door for anesthetic xenon recovery using Bio-MOFs

Behra Canturk, Zekiye Erarслан and Yeliz Gurdal\*



## RESEARCH PAPERS

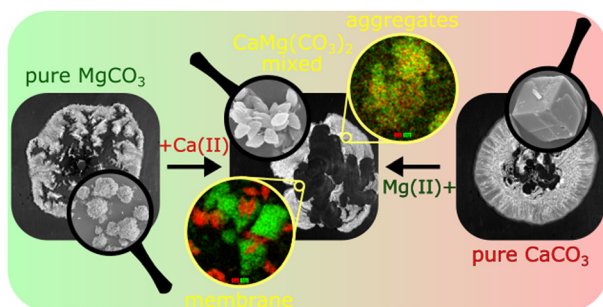
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### Analysis of the bonding in tetrahedrane and phosphorus-substituted tetrahedranes

Daniel Del Angel Cruz, Jorge L. Galvez Vallejo and Mark S. Gordon\*

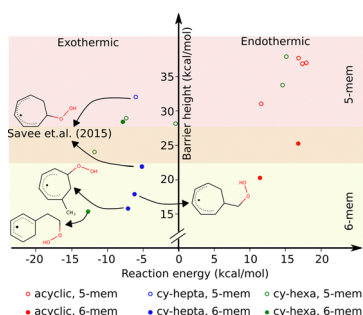
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### Synthesis and composition modification of precipitate tubes in a confined flow reactor

Kinga Bene, Edina Balog and Gábor Schuszter\*

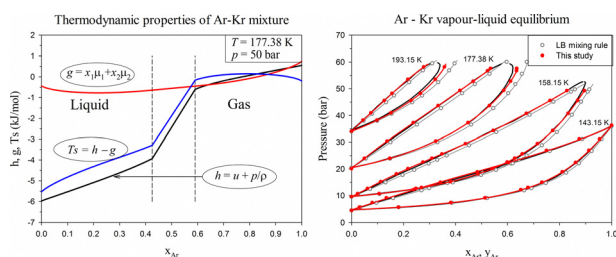
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### Stereo-electronic factors influencing the stability of hydroperoxyalkyl radicals: transferability of chemical trends across hydrocarbons and *ab initio* methods

Saurabh Chandra Kandpal, Kgalaleto P. Otukile, Shweta Jindal, Salini Senthil, Cameron Matthews, Sabyasachi Chakraborty, Lyudmila V. Moskaleva\* and Raghunathan Ramakrishnan\*

27321



### Thermodynamics of liquid and fluid mixtures from the kinetic Monte Carlo viewpoint

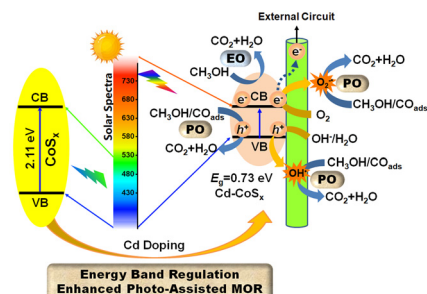
Eugene A. Ustinov



27331

### Metal organic framework-derived transition metal-doped $\text{CoS}_x$ nanocage for enhanced visible light-assisted methanol electrocatalytic oxidation

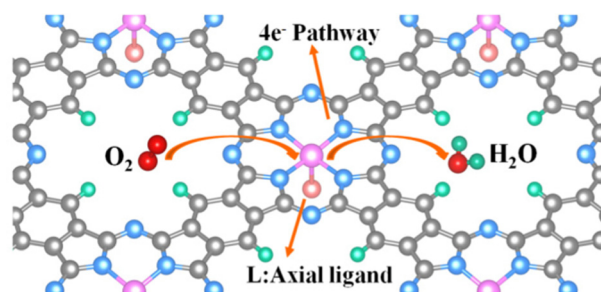
Meng Li, Quan Du, Guanfeng Li, Lei Qian\* and Ying Zeng



27342

### A theoretical study on the ORR electrocatalytic activity of axial ligand modified cobalt polyphthalocyanine

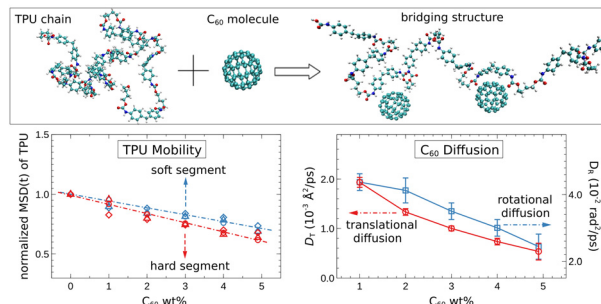
Guilin Wang, Xiaoli Yang, Ruiying Wang and Jianfeng Jia\*



27352

### Structural and dynamical properties of thermoplastic polyurethane/fullerene nanocomposites: a molecular dynamics simulations study

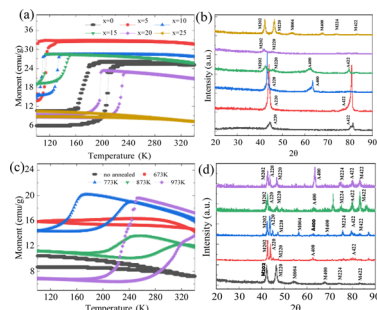
Jianxiang Shen, Xue Li,\* Ping Li and Baoqing Shentu\*



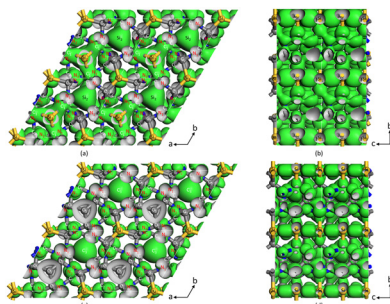
27364

### The effect of quenching and Mn substitution for Ni on the magnetic properties of $\text{Mn}_{25+x}\text{Ni}_{50-x}\text{Ga}_{25}$

Tianfeng Zhang, Lizhi Yi,\* Jiaohong Huang, Yingde Zhang, Yunli Xu, Ming Liu, Xiong He and Liqing Pan\*



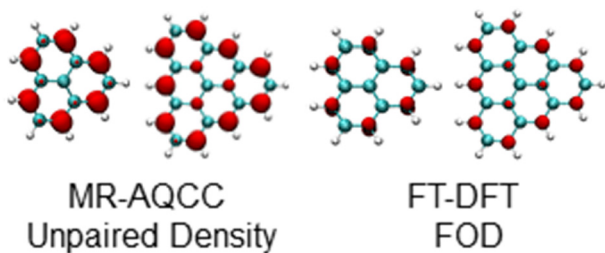
27373



### Hardness and electronic properties of Si–C–N structures

Shuai Chen, Xiaogang Guo, Hefei Li, Pan Ying, Rongxin Sun, Mengdong Ma, Yingju Wu, Lingjuan Hao, Dongli Yu, Julong He,\* Yufei Gao\* and Yongjun Tian

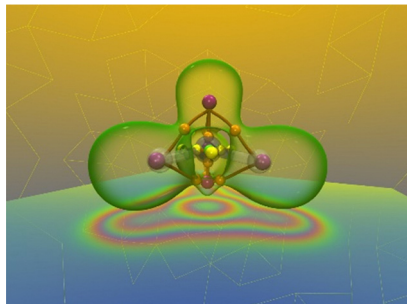
27380



### Polyradical character assessment using multireference calculations and comparison with density-functional derived fractional occupation number weighted density analysis

Reed Nieman, Jhonatas R. Carvalho, Bhumika Jayee, Andreas Hansen, Adelia J. A. Aquino, Miklos Kertesz and Hans Lischka\*

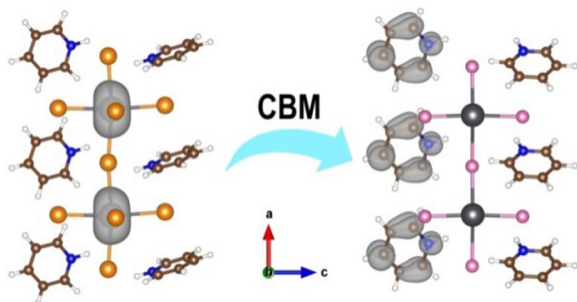
27394



### Revisiting the bonding evolution theory: a fresh perspective on the ammonia pyramidal inversion and bond dissociations in ethane and borazane

Leandro Ayarde-Henríquez,\* Cristian Guerra,\* Mario Duque-Noreña and Eduardo Chamorro\*

27409



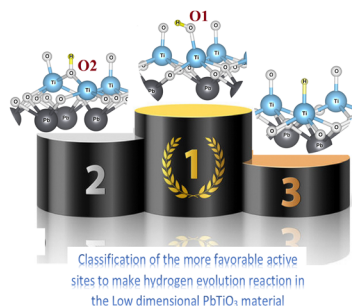
### Atomically thin two-dimensional hybrid perovskites using hydrophobic superalkali cations with tunable electron transition type

Tingwei Zhou\* and Bin Shao





27457

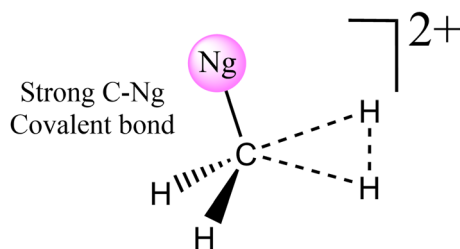


### Theoretical study of electrocatalytic properties of low-dimensional freestanding PbTiO<sub>3</sub> for hydrogen evolution reactions

Tarik Ouahrani,\* Reda M. Boufatah, Loubna Bendaoudi, Zeyneb Bedrane, Ángel Morales-García and Daniel Errandonea\*

27468

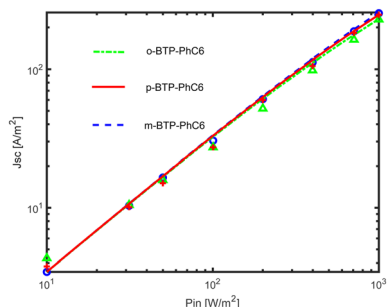
### Pentacoordinate Carbon



### Strong carbon – noble gas covalent bond and fluxionality in hypercoordinate compounds

Alejandro Vásquez-Espinal and Ricardo Pino-Rios\*

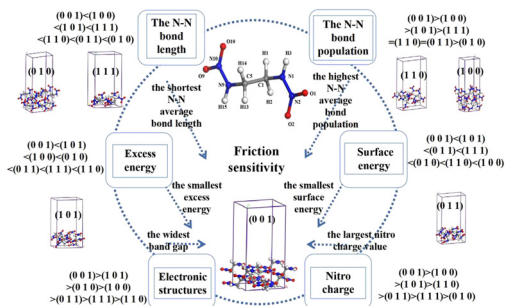
27475



### An analytical model for organic bulk heterojunction solar cells based on Saha equation for exciton dissociation

Jiu-Xun Sun,\* Hong-Chun Yang, Yang Li and Hai-Juan Cui

27488



### Theoretical study on the correlation between the structure, excess energy, surface energy, electronic structure, nitro charge, and friction sensitivity of N,N'-dinitroethylenediamine (EDNA)

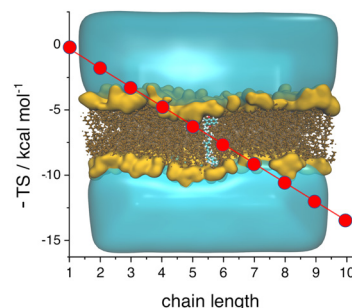
Hong-Yan Li, Yun-Dan Gan, Fu-Sheng Liu, Zheng-Tang Liu, Zhi-Xin Bai\* and Qi-Jun Liu\*



27498

### A trick of the tail: computing the entropic contribution to the energetics of quinone-protein unbinding

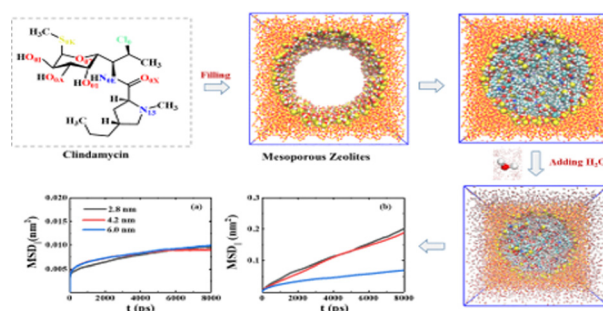
Jetmir Haxhija, Felix Guischar and Thorsten Koslowski\*



27506

### Molecular-scale insights into confined clindamycin in nanoscale pores of mesoporous silica

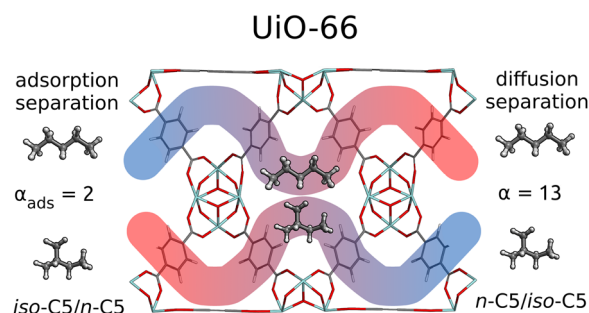
Xiaojun Wu,\* Haizhang Mu and Bihong Li



27516

### Mobility and separation of linear and branched C<sub>5</sub> alkanes in UiO-66 (Zr) probed by <sup>2</sup>H NMR and MD simulations

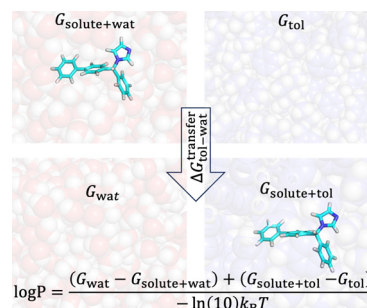
Alexander E. Khudozhnikov, Mikhail S. Plekhanov, Sergei S. Arzumanov, Daniil I. Kolokolov\* and Alexander G. Stepanov\*



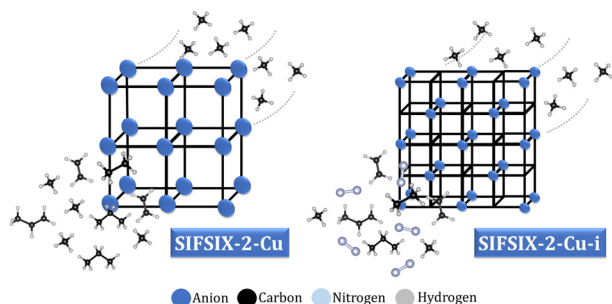
27524

### Energy-entropy multiscale cell correlation method to predict toluene–water log P in the SAMPL9 challenge

Hafiz Saqib Ali\* and Richard H Henchman\*



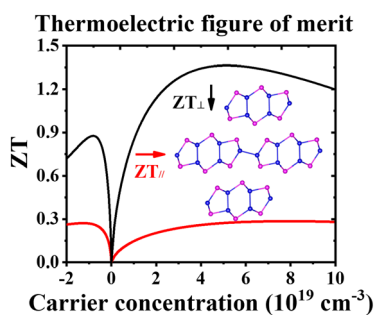
27532



### Dynamical and electronic properties of anion-pillared metal–organic frameworks for natural gas separation

Sabrina Grigoletto, Arthur Gomes dos Santos, Guilherme Ferreira de Lima and Heitor Avelino De Abreu\*

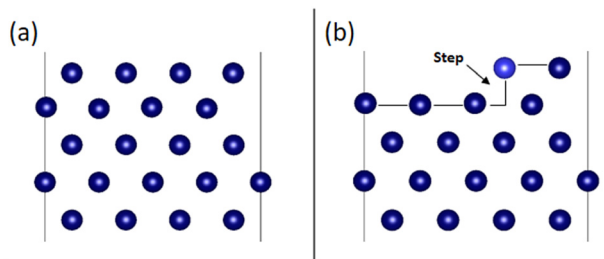
27542



### Anisotropic ductility and thermoelectricity of van der Waals GeAs

Xia Jiang, Tianqi Zhao and Dong Wang\*

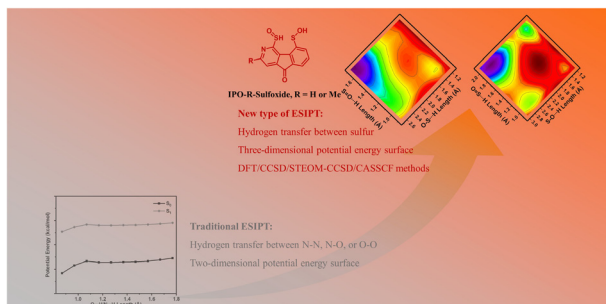
27553



### Exploring adsorption behavior of sulfur and nitrogen compounds on transition metal-doped Cu(100) surfaces: insights from DFT and MD simulations

Achraf Benbella,\* Hicham Jabraoui,\* Imane Matrane and M'hammed Mazroui

27566



### A brand-new type of excited-state proton transfer (ESIPT) molecule based on sulfoxide/sulfenic acid tautomerism

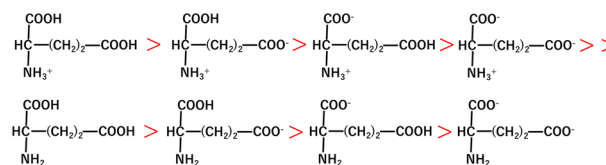
Rongchuan Su\* and Zhenmei Huang



27574

### DFT analysis of nitrogen isotopic reduction partition function ratios in proton exchange equilibria of glutamic acid species in water and its application to the estimation of nitrogen isotope fractionation

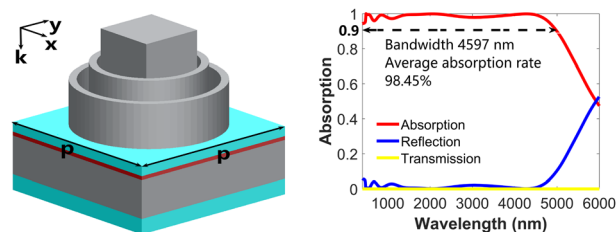
Takao Oi, Satoshi Yanase and Masaaki Musashi\*



27586

### An ultra-broadband solar absorber based on $\alpha$ -GST/Fe metamaterials from visible light to mid-infrared

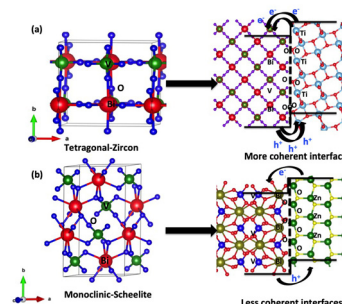
Yizhao Pan, Yuchang Li, Fang Chen,\* Shubo Cheng, Wenxing Yang, Boyun Wang, Zao Yi and Duanzheng Yao



27595

### Tetragonal-zircon $\text{BiVO}_4$ : a better polymorph for the formation of coherent type-II heterostructures for water splitting applications

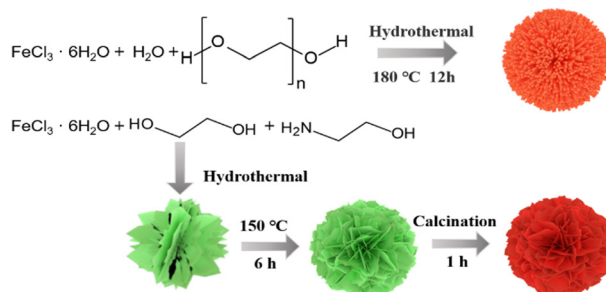
Rashmi, Md Majid and Sri Sivakumar\*



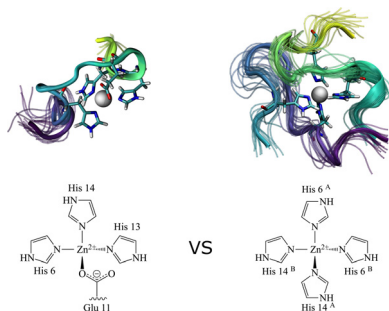
27606

### $\text{Fe}_2\text{O}_3$ for stable K-ion storage: mechanism insight into dimensional construction from stress distribution and micro-tomography

Haiting Shi, Qingqing Wu, Jinxi Bao, Shuaitong Liang, Yanli Hu, Ruiqi Shao,\* Shuo Wang, Jie Shi and Zhiwei Xu\*



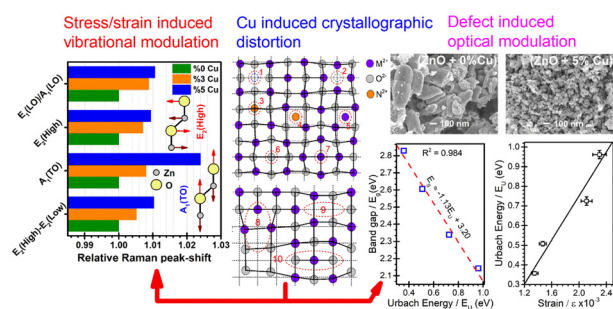
27618



## Rules governing metal coordination in $\text{A}\beta\text{-Zn(II)}$ complex models from quantum mechanical calculations

Julen Aduriz-Arrizabalaga, Jose M. Mercero, David De Sancho and Xabier Lopez\*

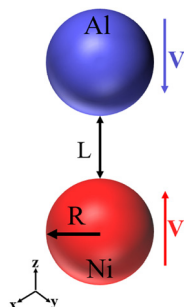
27628



## Influence of Cu induced crystallographic disorder on the optical and lattice vibrational properties of ZnO nanoparticles

Md. Abdullah Zubair,\* Tasnim Kamal Mouri and Mohammed Tareque Chowdhury

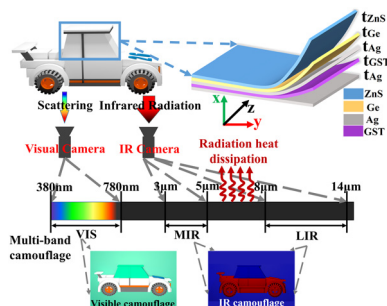
27654



## Deformation, damage, and reaction characteristics during the collision between Ni and Al nanoparticles

Kexin Zhu, Yifan Xie, Jian-Li Shao\* and Pengwan Chen

27668



## A tunable infrared emitter based on phase-changing material GST for visible-infrared compatible camouflage with thermal management

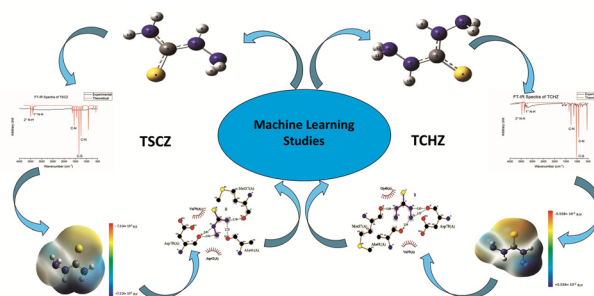
Qianlong Kang, Kai Guo\* and Zhongyi Guo\*



27677

### Spectroscopic characterization, molecular docking and machine learning studies of sulphur containing hydrazide derivatives

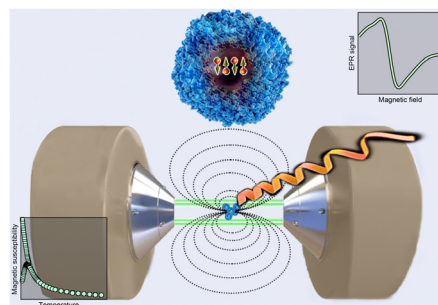
Soni Shukla, Poonam Rawat, Pulkit Sharma, Prince Trivedi, Faraz Ghous and Abha Bishnoi\*



27694

### In-depth magnetometry and EPR analysis of the spin structure of human-liver ferritin: from DC to 9 GHz

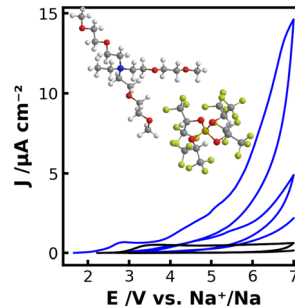
Lucia Bossoni, Jacqueline A. Labra-Muñoz, Herre S. J. van der Zant, Vera Čaluković, Anton Lefering, Ramon Egli\* and Martina Huber\*



27718

### Fluoroborate ionic liquids as sodium battery electrolytes

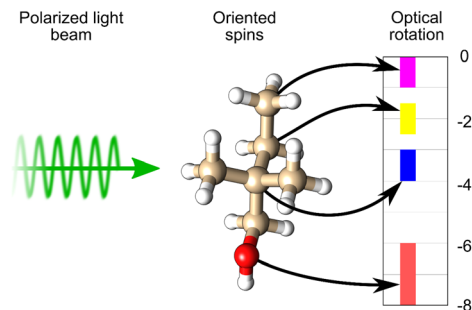
Dale T. Duncan, Samantha L. Piper, Maria Forsyth, Douglas R. MacFarlane and Mega Kar\*



27731

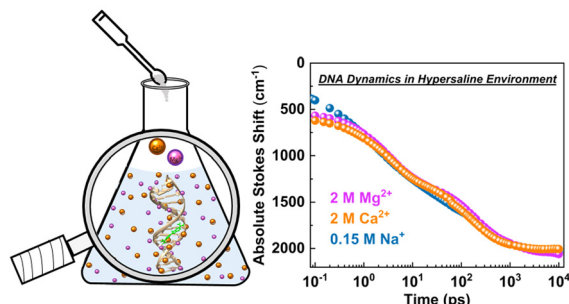
### Characteristic nuclear spin-induced optical rotation in oxygen-containing organic molecules

Eelis Kamula, Juha Vaara and Petr Štěpánek\*



## RESEARCH PAPERS

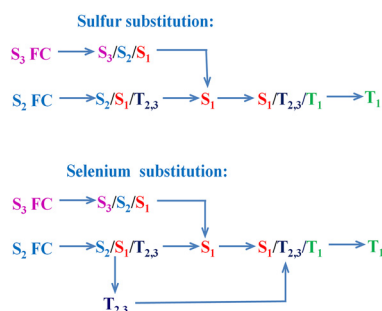
27744



### Unusual similarity of DNA solvation dynamics in high-salinity crowding with divalent cations of varying concentrations

Deepika Sardana,\* Parvez Alam, Kavita Yadav, Ndege Simisi Clovis, Pramod Kumar and Sobhan Sen\*

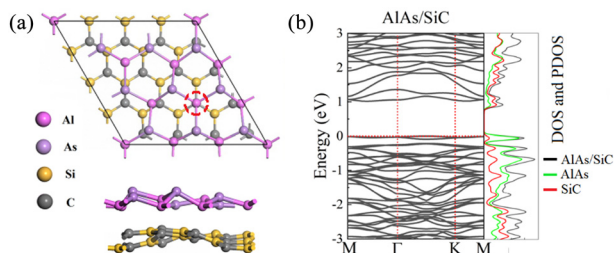
27756



### The impact of the chalcogen-substitution element and initial spectroscopic state on excited-state relaxation pathways in nucleobase photosensitizers: a combination of static and dynamic studies

Min Xie, Shuang-xiao Ren, Die Hu, Ji-meng Zhong, Jie Luo, Yin Tan, Yan-ping Li, Li-ping Si and Jun Cao\*

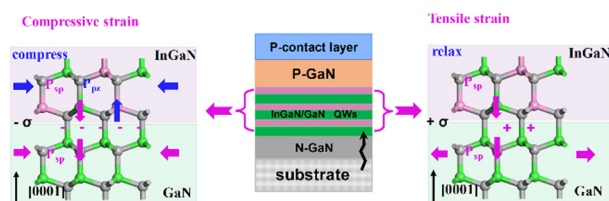
27766



### Effect of external electric field on the electronic properties of the AlAs/SiC van der Waals heterostructure

Zicheng Zhang, Changxin Wan, Heng Li, Chunsheng Liu, Lan Meng\* and Xiaohong Yan

27774



### Efficiency enhancement mechanism of piezoelectric effect in long wavelength InGaN-based LED

Li Liu, Qingqing Feng, Yu Zhang, Xiaolu Zhu, Lanli Chen\* and Zhihua Xiong\*

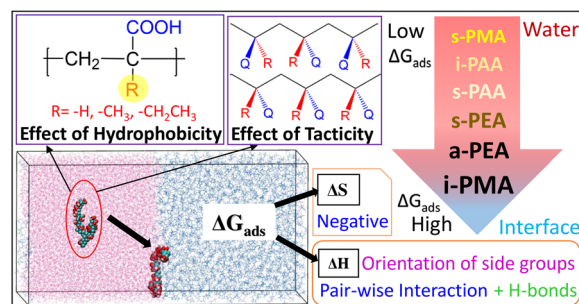


## RESEARCH PAPERS

27783

### Complex role of chemical nature and tacticity in the adsorption free energy of carboxylic acid polymers at the oil–water interface: molecular dynamics simulations

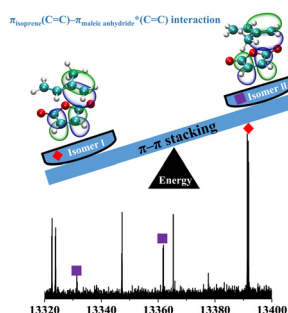
Raviteja Kurapati and Upendra Natarajan\*



27798

### Conformational equilibria and interaction preference in the complex of isoprene–maleic anhydride

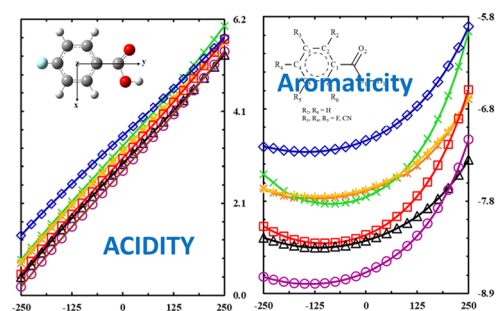
Tianyue Gao, Juncheng Lei, Siyu Zou, Chenxu Wang, Xuefang Xu\* and Qian Gou\*



27805

### Directionality and additivity effects of molecular acidity and aromaticity for substituted benzoic acids under external electric fields

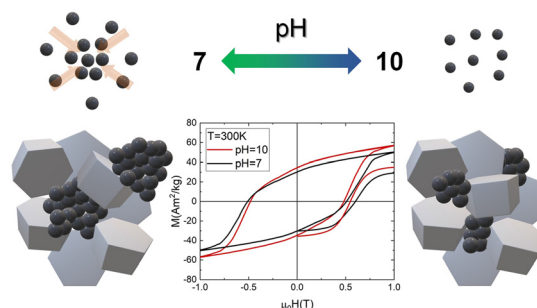
Meng Li, Xinjie Wan, Chunying Rong,\* Dongbo Zhao\* and Shubin Liu\*



27817

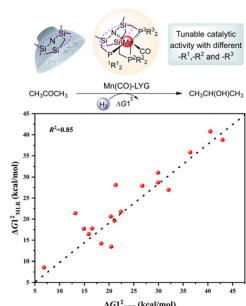
### Tunable particle-agglomeration and magnetic coupling in bi-magnetic nanocomposites

Pierfrancesco Maltoni,\* Miran Baričič, Gianni Barucca, Maria Chiara Spadaro, Jordi Arbiol, Nader Yaacoub, Davide Peddis\* and Roland Mathieu\*



## RESEARCH PAPERS

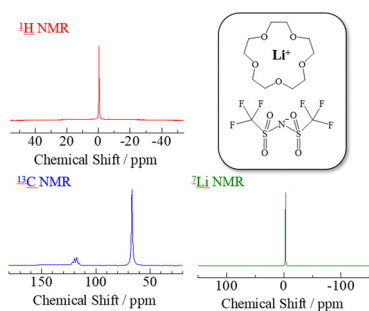
27829



**The theoretical design of manganese catalysts with a Si–N–Si–C–Si–C six-membered ring core-based bowl-shaped quadridentate ligand for the hydrogenation of C=O/C=N bonds**

Yunfan Yue, Tian Ma, Hexiang Qi, Yaqi Zhao, Xiaofan Shi, Yanhui Tang, Min Pu and Ming Lei\*

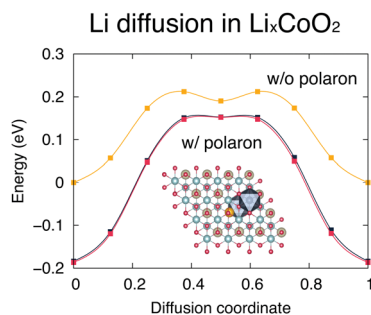
27836



**Solid state  $^1\text{H}$ ,  $^7\text{Li}$ , and  $^{13}\text{C}$  NMR studies on new ionic plastic crystals of crown ether–Li–TFSA complexes**

Akira Kobayashi, Jun Yamagami, Subham Ranjan, Satoshi Takamizawa and Hisashi Honda\*

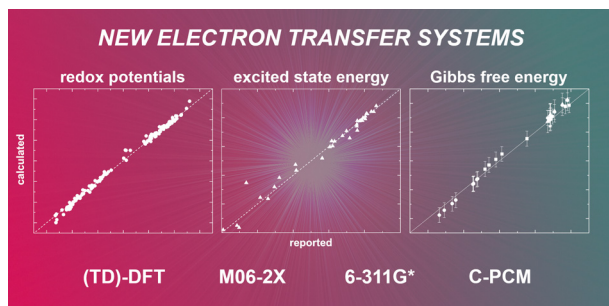
27848



**First-principles study on small polaron and Li diffusion in layered  $\text{LiCoO}_2$**

Seryung Ahn, Jiyeon Kim, Bongjae Kim and Sooran Kim\*

27854



**Full theoretical protocol for the design of metal-free organic electron donor–spacer–acceptor systems**

Amilcar Duque-Prata, Carlos Serpa and Pedro J. S. B. Caridade\*

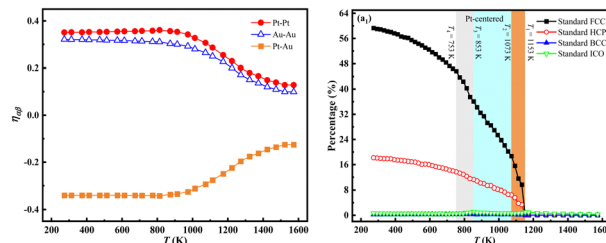


## RESEARCH PAPERS

27866

### Crystallization mechanism of the Pt<sub>50</sub>Au<sub>50</sub> alloy with grain boundary segregation during the solidification process

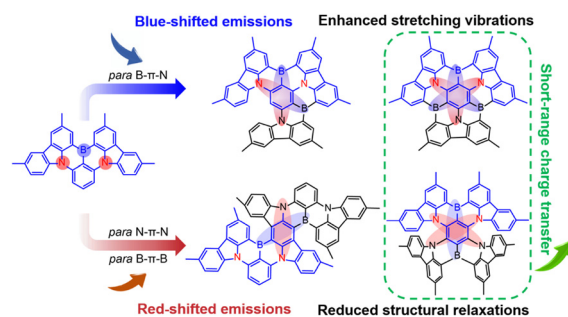
Q. H. Gao, P. F. Zou,\* Z. Y. Hou,\* J. B. Wu, Z. Wang and J. G. Wang



27877

### Achieving narrowband emissions with tunable colors for multiple resonance-thermally activated delayed fluorescence materials: effect of boron/nitrogen number and position

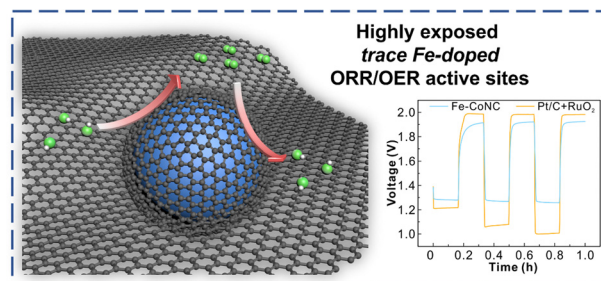
Ping Li, Yewen Zhang, Wenjing Li, Cefeng Zhou and Runfeng Chen\*



27885

### Enhancing the bifunctional oxygen reduction and evolution activity of CoNC by introducing a trace amount of Fe

Yongrong Sun, Zhikai Liu, Hailu Liu, Fayong Li, Lingfeng Li, Chunyu Du, Jia Li,\* Dong Xie\* and Guokang Han\*



## CORRECTION

27891

### Correction: Tuning the optical properties of the metal–organic framework UiO-66 via ligand functionalization

Marvin Treger, Adrian Hannebauer, Andreas Schaate, Jan L. Budde, Peter Behrens and Andreas M. Schneider\*

