

## IN THIS ISSUE

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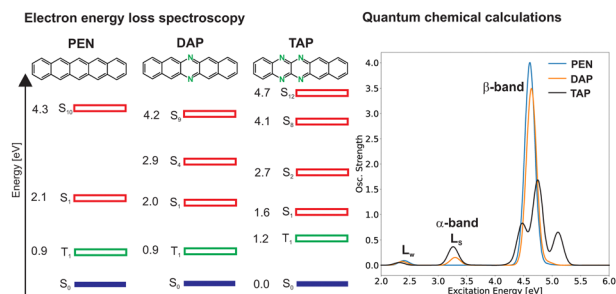
See Francesc Illas *et al.*,  
pp. 17116–17127.  
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*Phys. Chem. Chem. Phys.*,  
2023, 25, 17116.

## PERSPECTIVES

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### Influence of N-introduction on the electronic structure and properties of polyacenes: experiment and quantum chemistry in concert

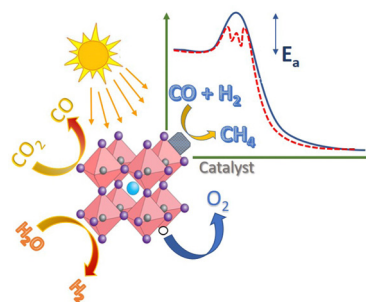
Andreas Dreuw\* and Petra Tegeder\*



17092

### Catalytic enhancement of production of solar thermochemical fuels: opportunities and limitations

Juan M. Coronado\* and Alicia Bayón



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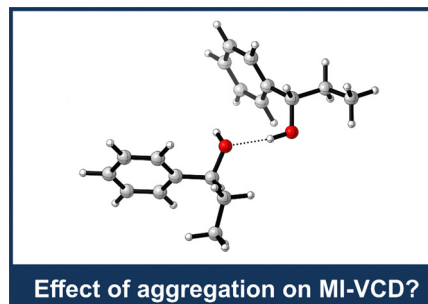


## COMMUNICATIONS

17107

**Matrix-isolation vibrational circular dichroism (VCD) spectroscopy of chiral 1-phenyl-1-propanol**

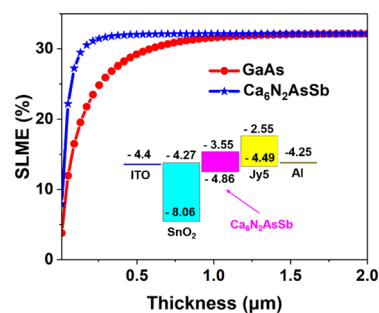
Corentin Grassin and Christian Merten\*



17112

**High-performance lead-free quaternary antiperovskite photovoltaic candidate  $\text{Ca}_6\text{N}_2\text{AsSb}$** 

Yanru Guo, Xue Liu, Huaxin Wang,\* Zhigang Zang and Ru Li\*

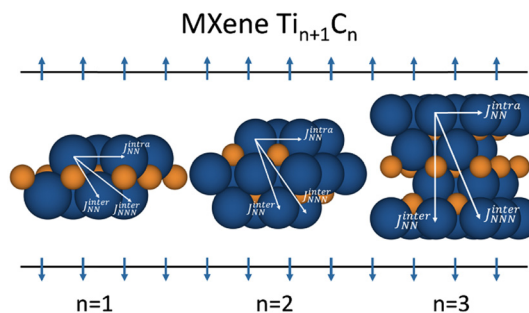


## RESEARCH PAPERS

17116

**How does thickness affect magnetic coupling in Ti-based MXenes**

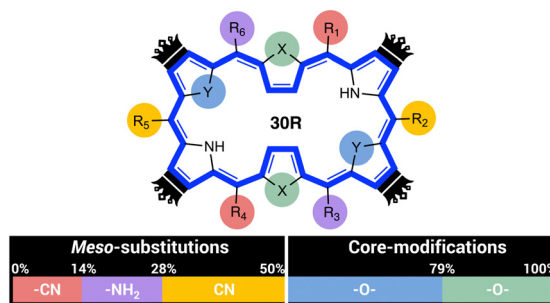
Néstor García-Romeral, Ángel Morales-García, Francesc Viñes, Ibério de P. R. Moreira and Francesc Illas\*



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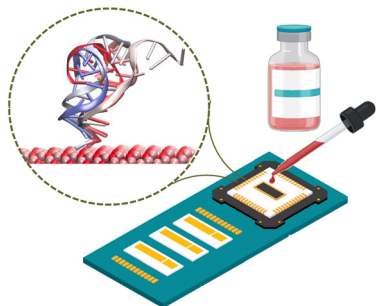
**Designing hexaphyrins for high-potential NLO switches: the synergy of core-modifications and meso-substitutions**

Eline Desmedt, David Smets, Tatiana Woller, Mercedes Alonso\* and Freija De Vleeschouwer\*



## RESEARCH PAPERS

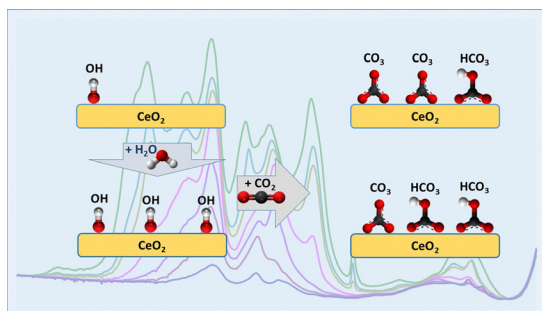
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### Utilization of DNA and 2D metal oxide interaction for an optical biosensor

Partha Kumbhakar, Indrani Das Jana, Subhadip Basu, Sandip Mandal, Saptarshi Banerjee, Subhanita Roy, Chinmayee Chowde Gowda, Anyesha Chakraborty, Ashim Pramanik, Pooja Lahiri, Basudev Lahiri, Amreesh Chandra, Pathik Kumbhakar, Arindam Mondal,\* Prabal K Maiti\* and Chandra Sekhar Tiwary\*

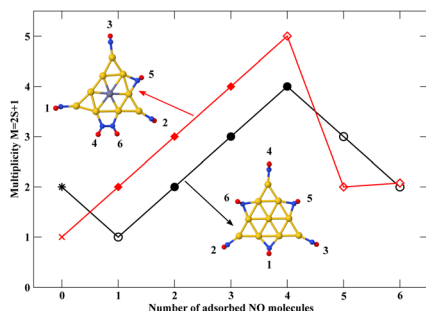
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### Capturing CO<sub>2</sub> by ceria and ceria–zirconia nanomaterials of different origin

D. Panayotov,\* V. Zdravkova, O. Lagunov, S. Andonova, I. Spassova, D. Nihtianova, G. Atanasova, N. Drenchev, E. Ivanova, M. Mihaylov and K. Hadjiivanov

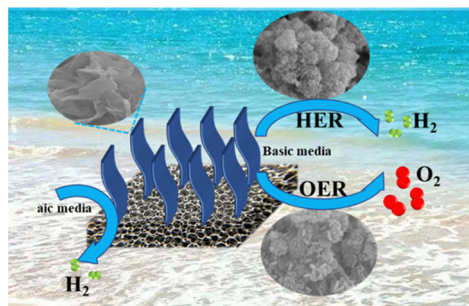
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### Adsorption of multiple NO molecules on Au<sub>10</sub><sup>−</sup> and Au<sub>9</sub>Zn<sup>−</sup> planar clusters. A comparative DFT study

Eva M. Fernández\* and Luis C. Balbás

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### Heterostructured Mo and Co-based phosphides as high-performance bifunctional electrocatalysts for overall water splitting

Hong Yang,\* Miao Yang, Tuoping Hu,\* Lijun Guo, Rongqian Meng, Yu Shi and Yajian Xu

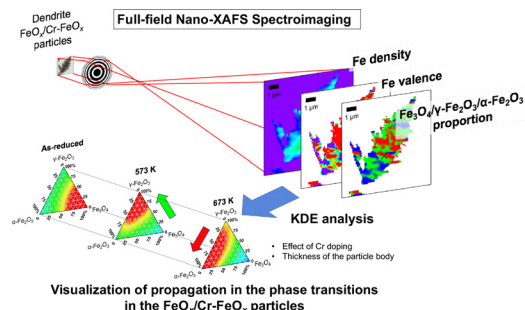


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# Oxidation and phase transfer of individual Cr-doped dendritic $\text{FeO}_x$ particles visualized by full-field nano-XAFS spectroimaging

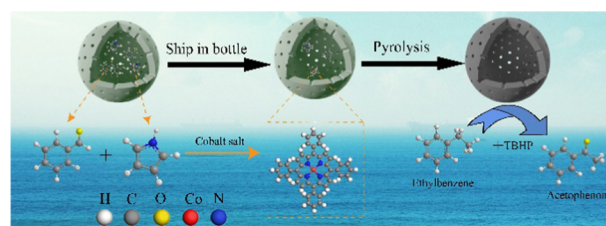
Nozomu Ishiguro,\* Hirosuke Matsui, Kohei Wakamatsu, Yoya Suzuki, Oki Sekizawa, Kiyofumi Nitta, Yasuko Terada, Tomoya Uruga and Mizuki Tada\*



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# In situ-synthesized Co and N-doped mesoporous hollow silica spheres for the selective oxidation of ethylbenzene

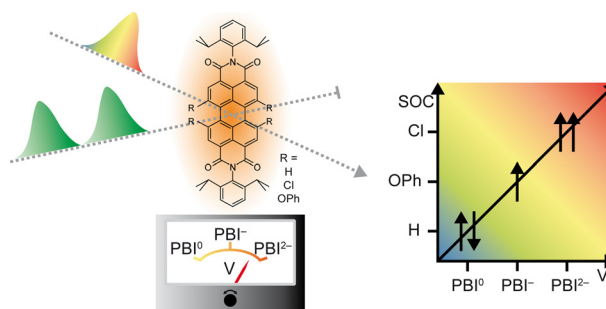
Yingying Lan, Chengfeng Yi and Zhigang Liu\*



17214

# Intersystem crossing of perylene bisimide neutral, radical anion, and dianion derivatives compared via ultrafast spectroelectrochemistry

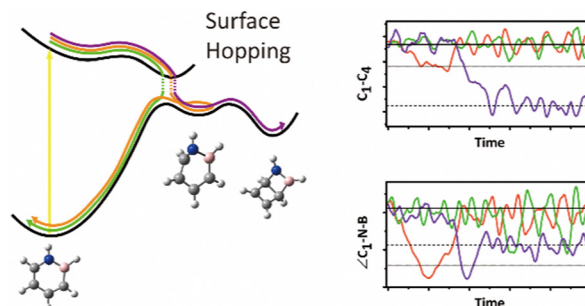
Julia Heitmüller, Rebecca Fröhlich, Rebecca Renner, Frank Würthner and Tobias Brixner\*



17230

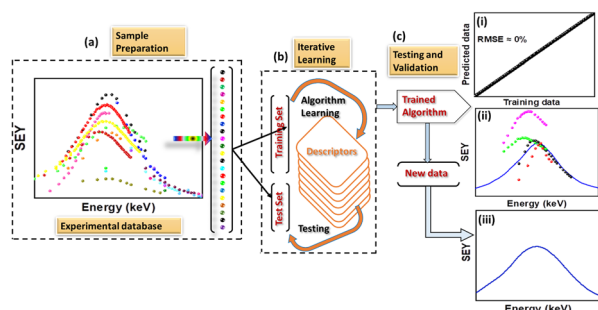
# Ultrafast photoisomerization mechanism of azaborine revealed by nonadiabatic molecular dynamics simulations

Sangmin Jeong, Eunji Park, Joonghan Kim\* and Kyung Hwan Kim\*



## RESEARCH PAPERS

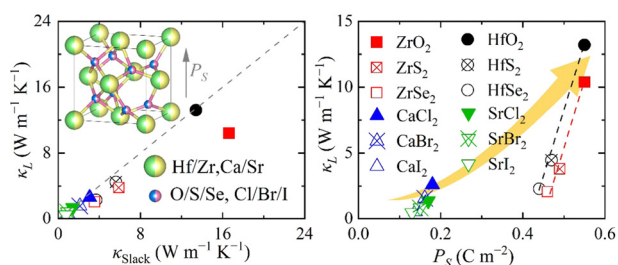
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## Exploring the absolute yield curve of secondary electrons using machine learning methods

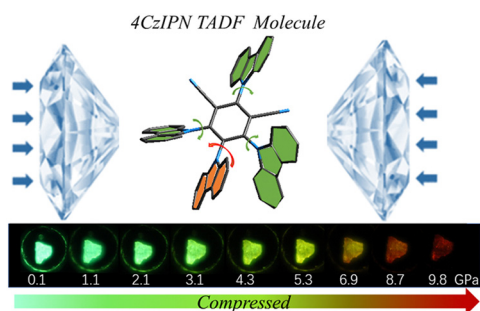
Mehnaz, Bo Da\* and Z. J. Ding\*

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First-principles study of thermal transport properties in ferroelectric HfO<sub>2</sub> and related fluorite-structure ferroelectrics

Shenglong Zhang, Shilei Yi, Jia-Yue Yang, Jian Liu\* and Linhua Liu\*

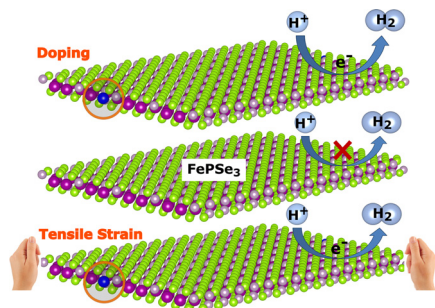
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## Pressure-shortened delayed fluorescence lifetime of solid-state thermally activated delayed fluorescent 4CzIPN: the structure evolution

Yarong Gu,\* Xuening Sun, Min Wu and Kai Wang

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From the single-atom limit to the mixed-metal phase: finding the optimum condition for activating the basal plane of a FePSe<sub>3</sub> monolayer towards HER

Megha and Prasenjit Sen\*

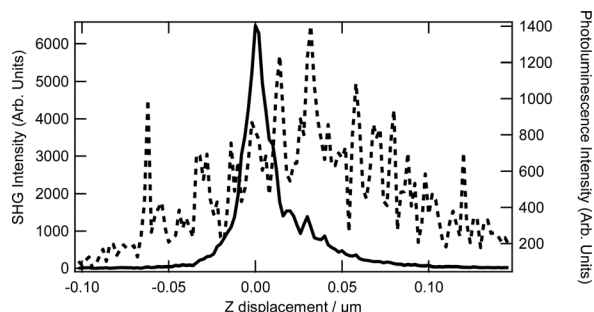


## RESEARCH PAPERS

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**Combining second harmonic generation and multiphoton excited photo-luminescence to investigate TiO<sub>2</sub> nanoparticle powders**

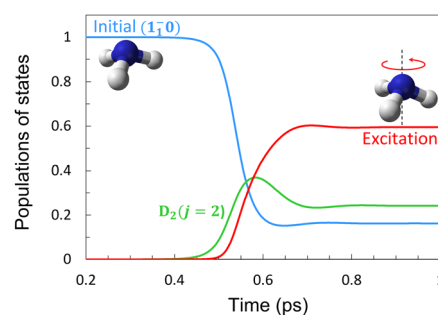
Christian Jonin,\* Estelle Salmon, Faheem Ahmed, Mohammed Benali Kanoun, Chawki Awada\* and Pierre-Francois Brevet



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**Mixed quantum/classical theory for rotational energy exchange in symmetric-top-rotor + linear-rotor collisions and a case study of the ND<sub>3</sub> + D<sub>2</sub> system**

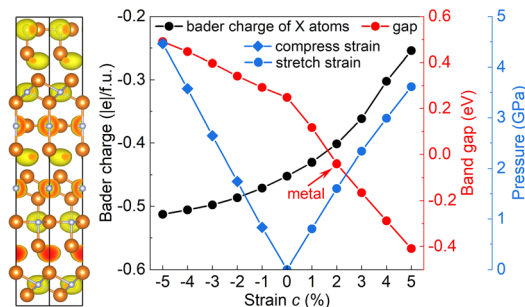
Carolyn Joy, Bikramaditya Mandal, Dulat Bostan and Dmitri Babikov\*



17300

**Transition from semiconductor to conductor of a Mg<sub>2</sub>N electride induced by strain**

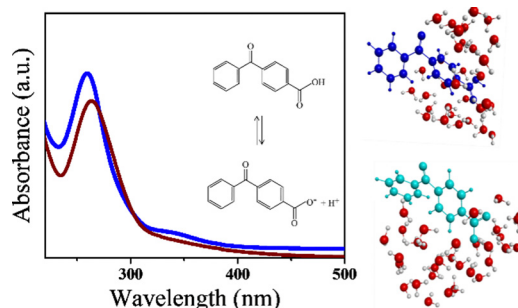
Gui Wang, Yongle Zhong, Yiguo Xu, Zhengfang Qian, Jingwen Jiang\* and Zhuang Ma\*



17306

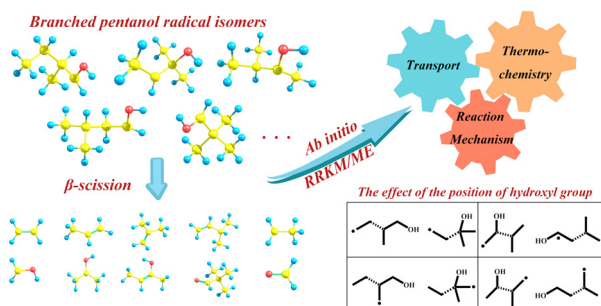
**pH Dependence of the speciation and optical properties of 4-benzoylbenzoic acid**

Natalia Karimova, Onita Alija, Stephanie L. Mora García, Vicki H. Grassian, R. Benny Gerber and Juan G. Navea\*



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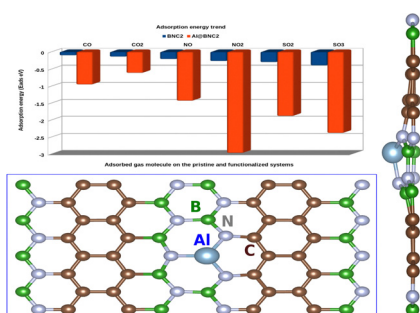
17320



### Theoretical investigation on isomerization and decomposition reactions of pentanol radicals-part I: branched pentanol isomers

Yueying Liang, Yuxiang Zhu, Jintao Chen, Xingcai Lu\* and Chong-Wen Zhou\*

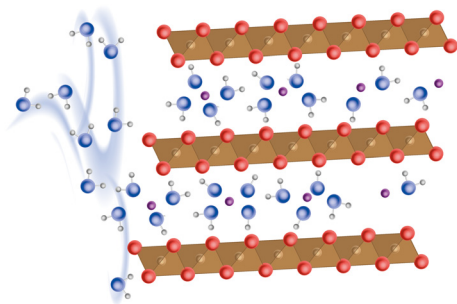
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### Adsorption mechanism of different toxic gases onto pristine BNC<sub>2</sub> and Al-doped BNC<sub>2</sub> monolayers

Poonam Chalase, Swapnil Deshpande, Sandip Kumavat and Mrinalini Deshpande\*

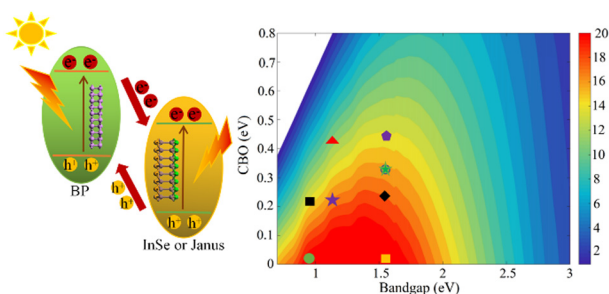
17352



### Temperature-resolved nanoscale hydration of a layered manganese oxide

N. Tan Luong, Hanna Oderstad, Michael Holmboe and Jean-François Boily\*

17360



### 2D layered BP/InSe and BP/Janus In<sub>2</sub>SeX (X = S or Te) type-II van der Waals heterostructures for photovoltaics: insight from first-principles calculations

Kai Cheng,\* Jinke Xu, Xu Guo, Sandong Guo and Yan Su\*

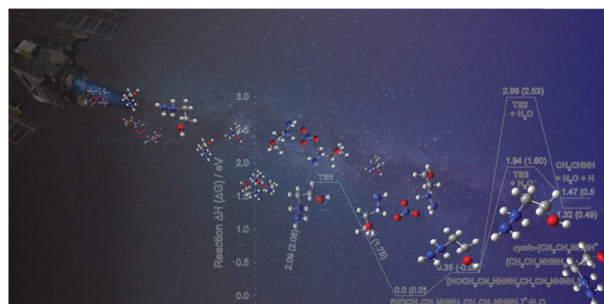


## RESEARCH PAPERS

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# Formation and fragmentation of 2-hydroxyethylhydrazinium nitrate (HEHN) cluster ions: a combined electrospray ionization mass spectrometry, molecular dynamics and reaction potential surface study

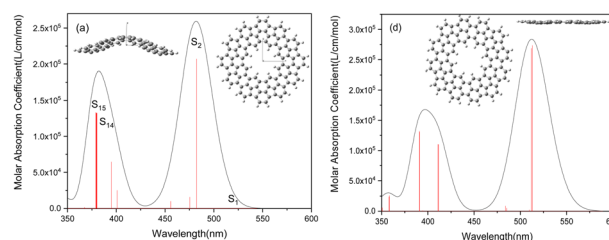
Wenjing Zhou, Jianbo Liu,\* Steven D. Chambreau and Ghanshyam L. Vaghjiani



17385

# Planar $\pi$ -extended all-armchair edge topological cycloparaphenylenes

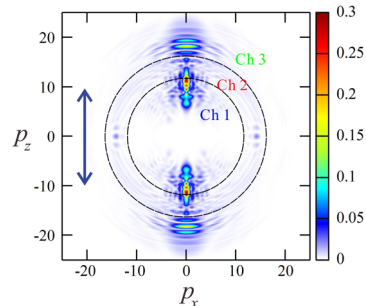
Ning Li and Mengtao Sun\*



17397

# Directly revealing the geometric phase effect of dissociative $D_2^+$ by two-color strong field photodissociation

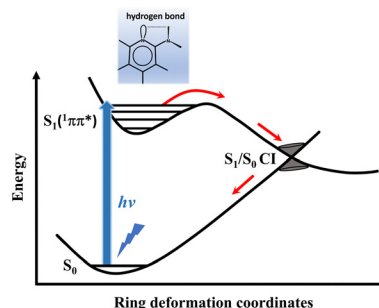
Sun Zhaopeng\* and Liu Yunquan\*

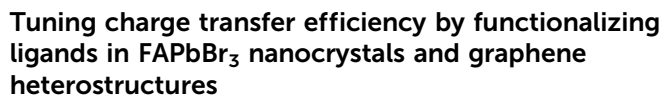


17403

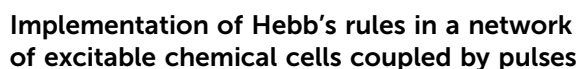
# Excitation wavelength dependent $S_1$ -state decay dynamics of 2-aminopyridine and 3-aminopyridine

Baihui Feng, Dongyuan Yang,\* Yanjun Min, Qinghua Gao, Benjie Fang, Guorong Wu\* and Xueming Yang

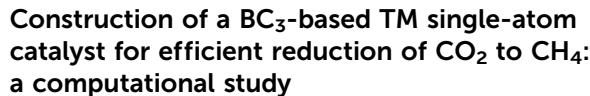




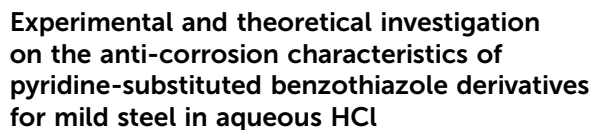
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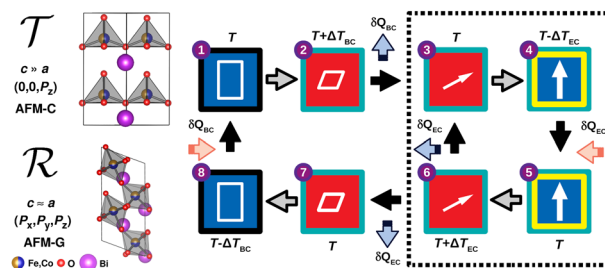
17072 | *Phys. Chem. Chem. Phys.*, 2023, **25**, 17063–17078

## RESEARCH PAPERS

17450

## Colossal room-temperature electrocaloric strength aided by hydrostatic pressure in lead-free multiferroic solid solutions

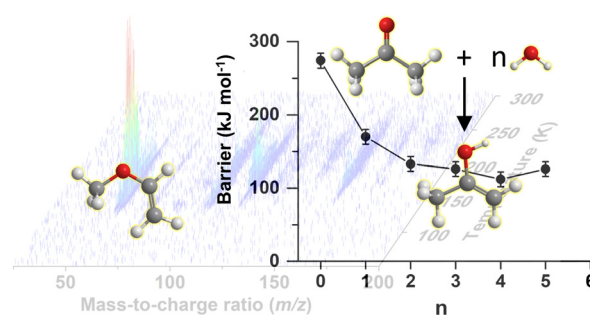
César Menéndez, Riccardo Rurali and Claudio Cazorla\*



17460

Synthesis of interstellar propen-2-ol ( $\text{CH}_3\text{C}(\text{OH})\text{CH}_2$ ) – the simplest enol tautomer of a ketone

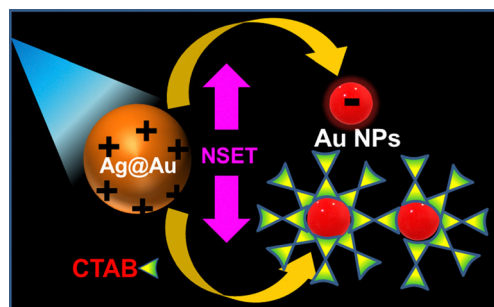
Jia Wang, Anatoliy A. Nikolayev, Chaojiang Zhang, Joshua H. Marks, Valeriy N. Azyazov, André K. Eckhardt\*, Alexander M. Mebel\* and Ralf I. Kaiser\*



17470

## Understanding the mechanism of the energy transfer process from non-plasmonic fluorescence bimetallic nanoparticles to plasmonic gold nanoparticles

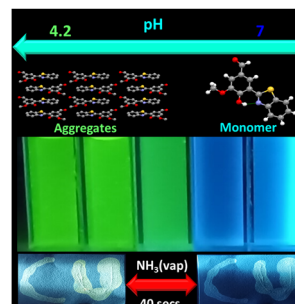
Amit Akhuli, Naupada Preeyanka, Debabrata Chakraborty and Moloy Sarkar\*



17482

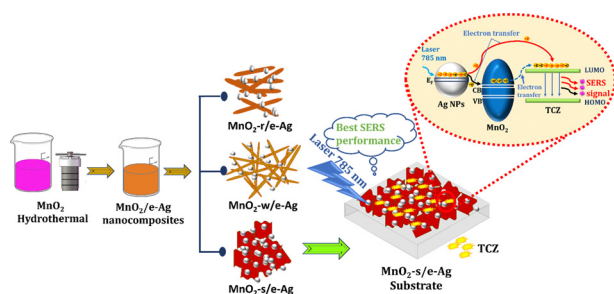
## Structural isomerism induces pH dependent AIE-coupled ESIPT: an in-depth spectroscopic exploration with application in amine vapor sensing

Arghyadeep Bhattacharyya, Viki Bhakta and Nikhil Guchhait\*



## RESEARCH PAPERS

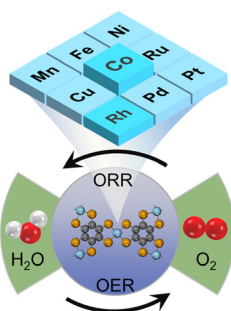
17496



**A manganese dioxide–silver nanostructure-based SERS nanoplatfor for ultrasensitive tricyclazole detection in rice samples: effects of semiconductor morphology on charge transfer efficiency and SERS analytical performance**

Dao Thi Nguyet Nga, Quan Doan Mai, Nguyen Le Nhat Trang, Minh Khanh Pham, Nguyen Quang Hoa, Vu Dinh Lam, Hoang Van Tuan, Ha Anh Nguyen\* and Anh-Tuan Le\*

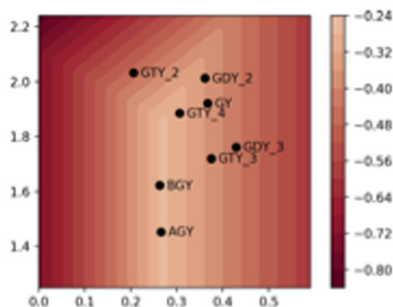
17508



**Two-dimensional metal–organic frameworks as bifunctional electrocatalysts for the oxygen evolution reaction and oxygen reduction reaction (OER/ORR): a theoretical study**

Feifei Xu, Zhixiao Gao, Zhencui Ge, Hao Ma, Hao Ren, Houyu Zhu, Yuhua Chi, Wenye Guo and Wen Zhao\*

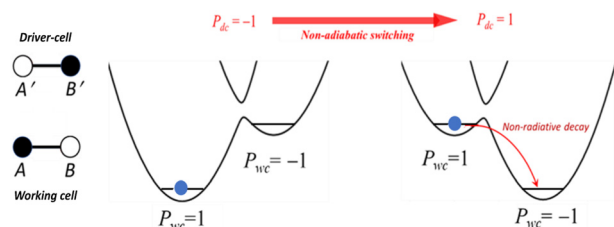
17515



**What governs the electrocatalytic N<sub>2</sub> reduction activity of sp-hybridized boron?**

Yongfei Ji,\* Yungan Huang, Gang Wang, Paiyong Liu and Wei quan Cai

17526



**In the quest for an optimal parametric regime of nonadiabatic switching ensuring low heat release in conjunction with high polarizability of mixed-valence molecular dimers**

Andrew Palii,\* Valeria Belonovich and Boris Tsukerblat\*

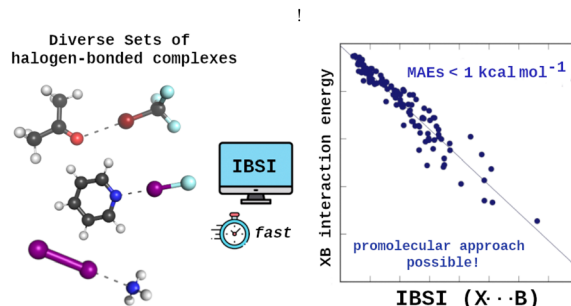


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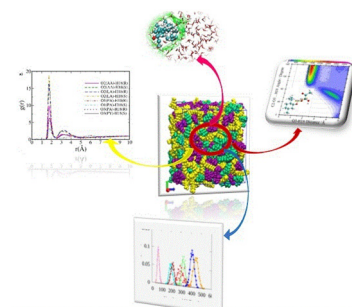
17535

**Intrinsic bond strength index as a halogen bond interaction energy predictor**

Ona Šivickytė and Paulo J. Costa\*



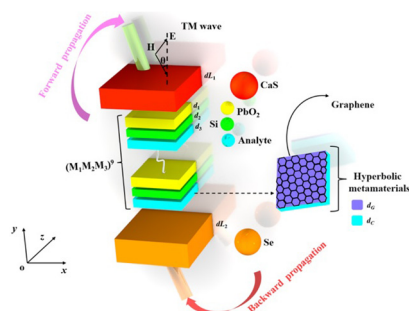
17547

**Assessment of the properties of natural-based chiral deep eutectic solvents for chiral drug separation: insights from molecular dynamics simulation**Parisa Jahanbakhsh-Bonab, Gholamreza Pazuki,\*  
Jaber Jahanbin Sardroodi and Seyed Mohsen Dehnavi

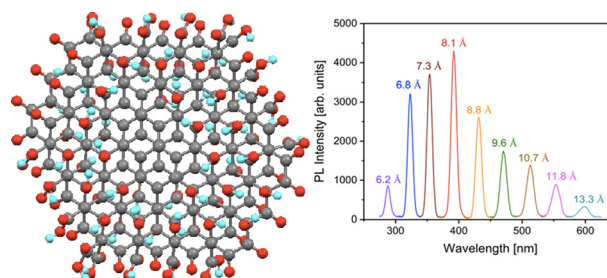
17558

**A multi-physical quantity sensor based on a layered photonic structure containing layered graphene hyperbolic metamaterials**

Jie Xu, Zhao Tang, You Ran Wu and Hai Feng Zhang\*

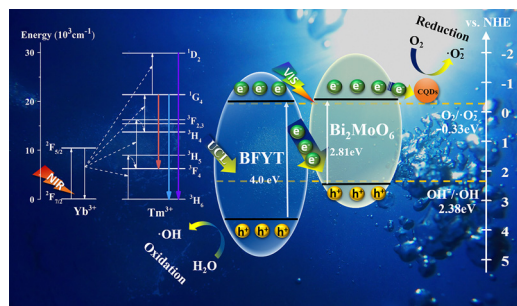


17571

**Uncommon 2D diamond-like carbon nanodots derived from nanotubes: atomic structure, electronic states, and photonic properties**D. W. Boukhvalov,\* D. A. Zatsepin, Yu. A. Kuznetsova,  
V. I. Pryakhina and A. F. Zatsepin

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17583

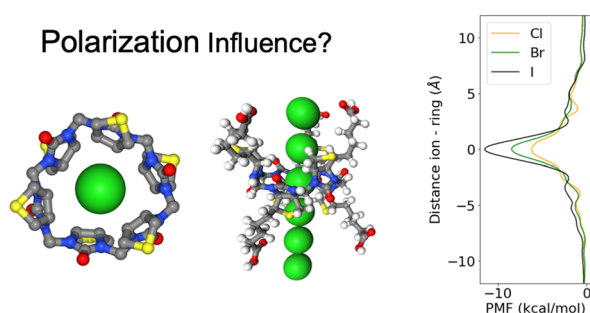


### Synergistic effects of rare earth doping and carbon quantum dots on BiOF/Bi<sub>2</sub>MoO<sub>6</sub> heterojunctions for enhanced visible-near-infrared photocatalysis

Wen Liu, Yan Cheng, Sui Jin, Kexin Wang, Junqi Ma, Baijie Guan, Ziye Ren, Tianya Tan\* and Jiwei Wang\*

17596

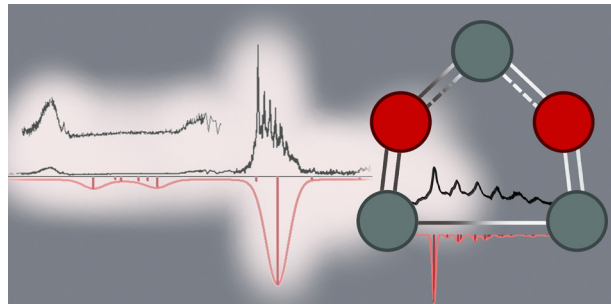
### Polarization Influence?



### 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\*

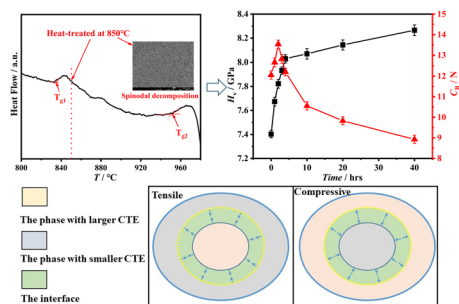
17609



### Photochemical properties of a potential interstellar dust precursor: the electronic spectrum of Si<sub>3</sub>O<sub>2</sub><sup>+</sup>

Taarna Studemund, Kai Pollow, Marko Förstel and Otto Dopfer\*

17619



### Tuning the hardness and crack resistance through liquid-liquid phase separation in an aluminosilicate glass

Feiyue Xia, Xiaowei Wang, Yadan Wang, Xiaoming Ren, Ang Qiao and Haizheng Tao\*

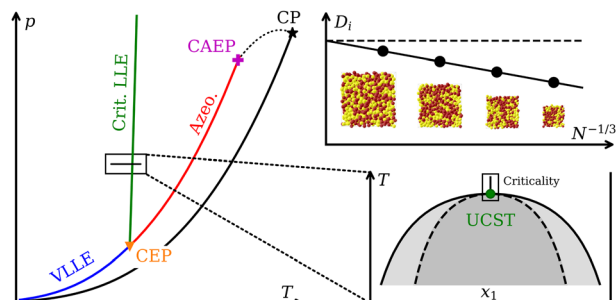


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17627

### Phase equilibria of symmetric Lennard-Jones mixtures and a look at the transport properties near the upper critical solution temperature

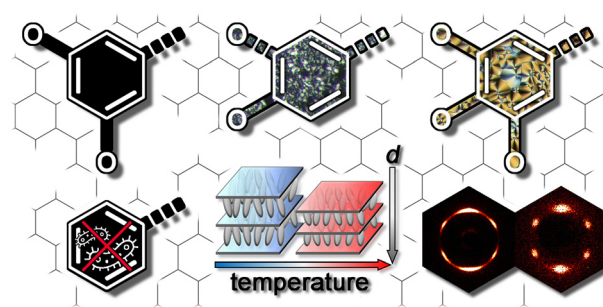
Ivan Antolović, Jens Staubach, Simon Stephan and Jadran Vrabec\*



17639

### Does thermotropic liquid crystalline self-assembly control biological activity in amphiphilic amino acids? – tyrosine ILCs as a case study

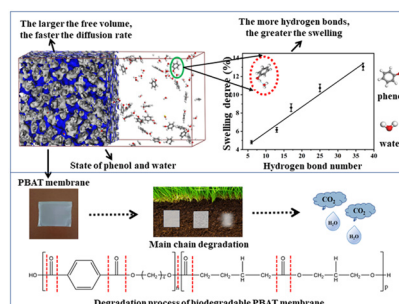
Marco André Grunwald, Selina Emilie Hagenlocher, Larissa Turkanovic, Soeren Magnus Bauch, Sebastian Benedikt Wachsmann, Luca Alexa Altevogt, Max Ebert, Julius Agamemnon Knöller, Aileen Rebecca Raab, Finn Schulz, Mohamed A. Kolmangadi, Anna Zens, Patrick Huber, Andreas Schönhals, Ursula Bilitewski\* and Sabine Laschat\*



17657

### Application of a biodegradable poly(butylene adipate-co-terephthalate) membrane for phenol pervaporation recovery

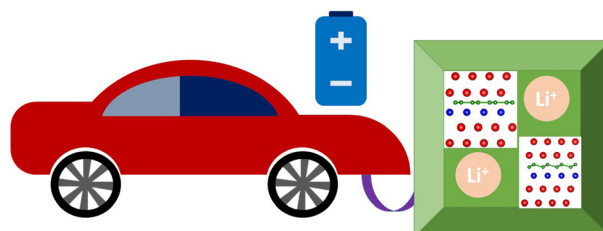
Meng Zhang, Qian Xu, Changlin Liu, Xiaowei An, Zhonglin Zhang, Xiao Du, Ping Li, Jianbing Wu and Xiaogang Hao\*



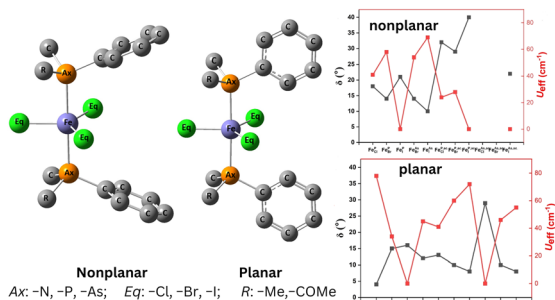
17667

### Monolayer molybdenum diborides containing flat and buckled boride layers as anode materials for lithium-ion batteries

Gayatree Barik and Sourav Pal\*



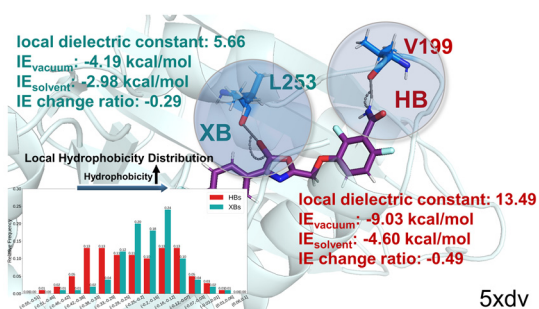
17680



## Spin-state energetics and magnetic anisotropy in penta-coordinated Fe(III) complexes with different axial and equatorial ligand environments

Shalini Joshi, Sabyasachi Roy Chowdhury and  
Sabyashachi Mishra\*

17692



## Preferred microenvironments of halogen bonds and hydrogen bonds revealed using statistics and QM/MM calculation studies

Liping Zhou, Jintian Li, Yulong Shi, Leyun Wu,  
Weiliang Zhu\* and Zhijian Xu\*