

## IN THIS ISSUE

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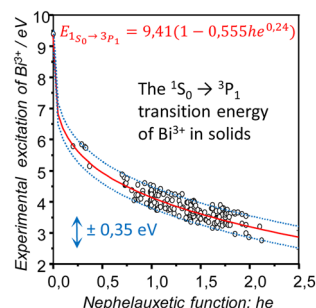
See J. Palaudoux *et al.*, pp. 11085–11092.  
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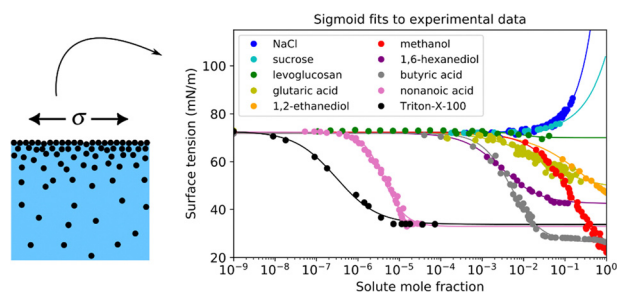
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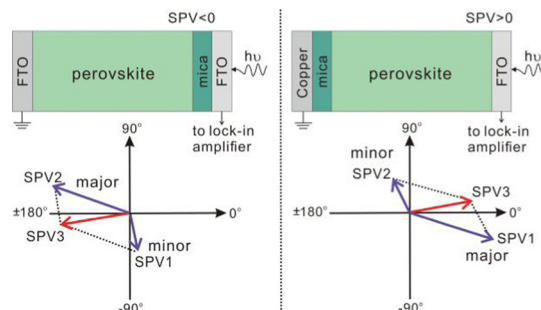


## COMMUNICATIONS

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### Exploring charge behavior at the terminal surface and charge separation interface of organo-lead perovskite using *in situ* surface photovoltage spectroscopy

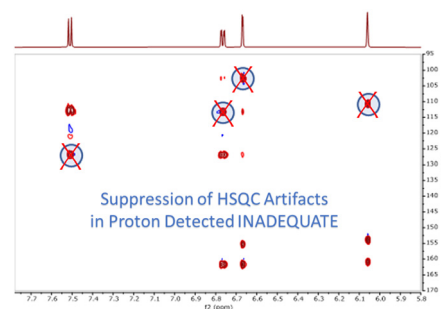
Fan Wu,\* Kaidong Zhan, Tiansheng Zhang, Ronghua Jian and Quinn Qiao\*



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### Origin and remedy for HSQC artifacts in proton-detected INADEQUATE spectra

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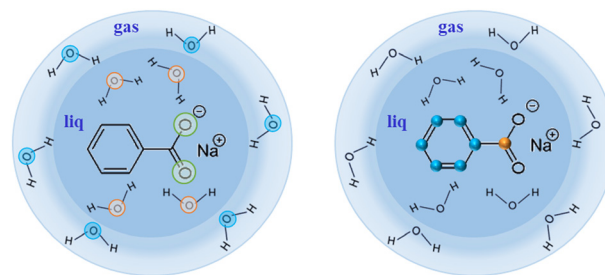


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### First (e,e) coincidence measurements on solvated sodium benzoate in water using a magnetic bottle time-of-flight spectrometer

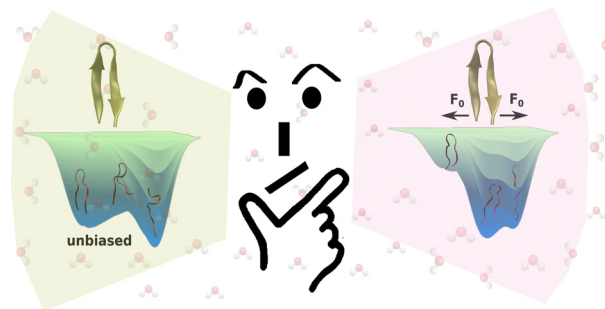
L. Huart, M. Fournier, R. Dupuy, R. Vacheresse, M. Mailhot, D. Cubaynes, D. Céolin, M. A. Hervé du Penhoat, J. P. Renault, J.-M. Guigner, A. Kumar, B. Lutet-Toti, J. Bozek, I. Ismail, L. Journal, P. Lablanquie, F. Penent, C. Nicolas and J. Palaudoux\*



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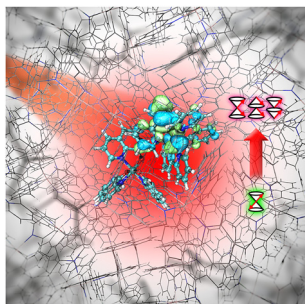
### Multifaceted folding–unfolding landscape of the TrpZip2 $\beta$ -hairpin and the role of external sub-piconewton mechanical tensions

Nayana Edavan Chathoth, Aparna G Nair and Padmesh Anjukandi\*



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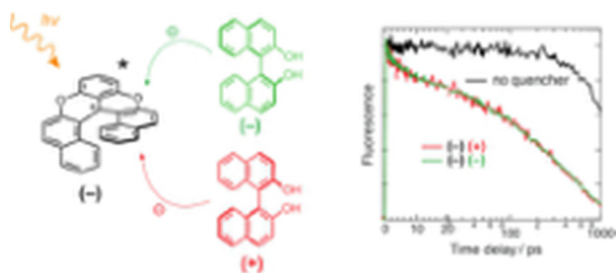
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### Crystalline matrix-activated spin-forbidden transitions of engineered organic crystals

Heming Zhang, Lianbao Ke, Yufang Nie, Zhengqian Tu, Jiaxuan Wang, Semion K. Saikin, Hai Bi\* and Yue Wang

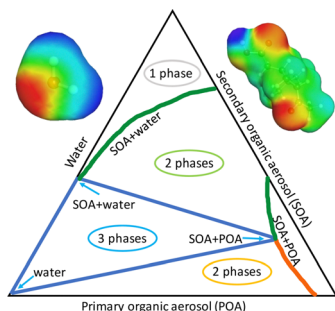
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### Looking for chiral recognition in photoinduced bimolecular electron transfer using ultrafast spectroscopy

Pragya Verma, Christoph Nançoz, Johann Bosson, Géraldine M. Labrador, Jérôme Lacour and Eric Vauthey\*

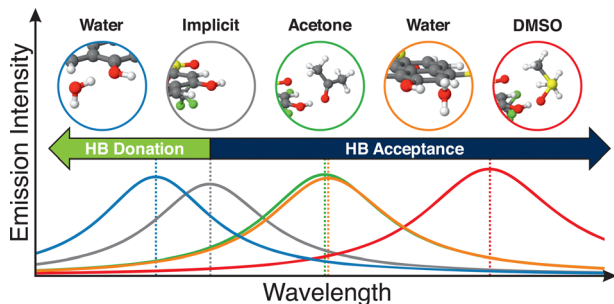
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Noora Hyttinen

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Niklas Sülzner\* and Christof Hättig

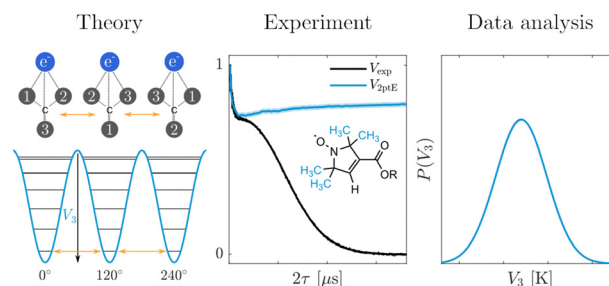


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### Quantifying methyl tunneling induced (de)coherence of nitroxides in glassy *ortho*-terphenyl at low temperatures

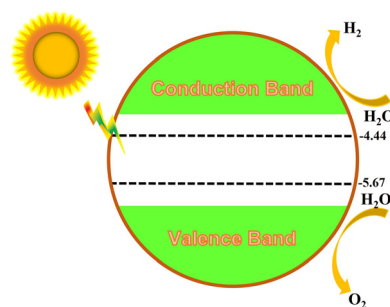
Andrea Eggeling, Janne Soetbeer,  
Luis Fábregas-Ibáñez, Daniel Klose and  
Gunnar Jeschke\*



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### The versatile characteristics of *Ars*/SGaInS van der Waals heterostructures

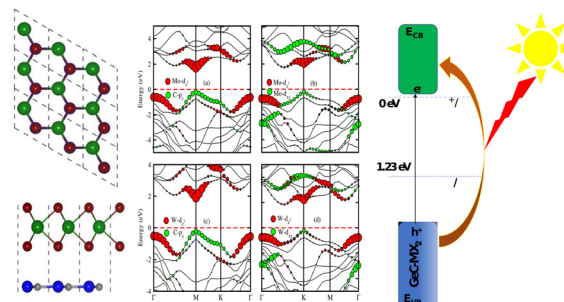
Iqtidar Ahmad, Anwar Ali, Ismail Shahid, Rawaid Ali,  
Wei Xiong, Lei Gao\* and Jinming Cai\*



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### A first principles study of structural and optoelectronic properties and photocatalytic performance of GeC–MX<sub>2</sub> (M = Mo and W; X = S and Se) van der Waals heterostructures

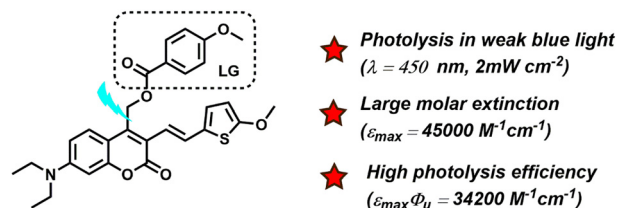
Tahir Wahab,\* Yun Wang and Antonio Cammarata\*



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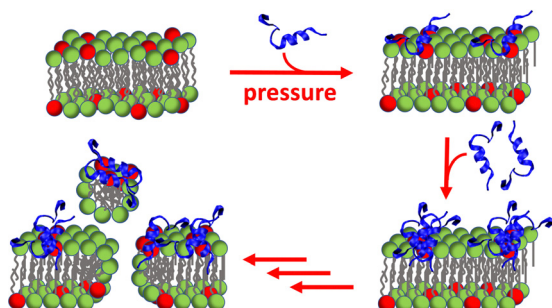
### Visible-light activatable coumarin-based phototriggers for fluorescence imaging with ultra-high photolysis efficiency

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Tuan Liu, Zhiqiang Wang, Xinyi Huang, Qiuning Lin,  
Xueqing Gong, Yi Yang and Linyong Zhu\*



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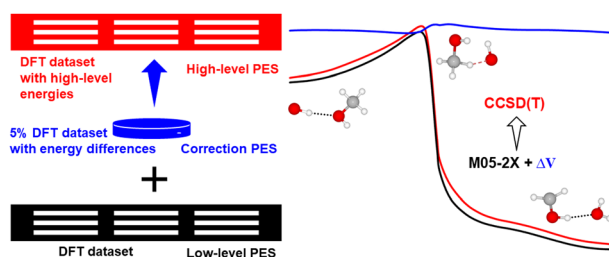
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### High pressure treatment promotes the deteriorating effect of cationic antimicrobial peptides on bacterial membranes

Simon Kriegler, Michel W. Jaworek, Rosario Oliva\* and Roland Winter\*

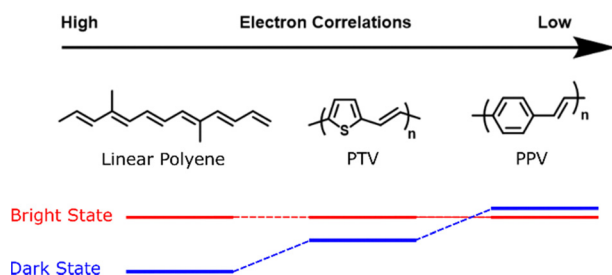
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Kaisheng Song and Jun Li\*

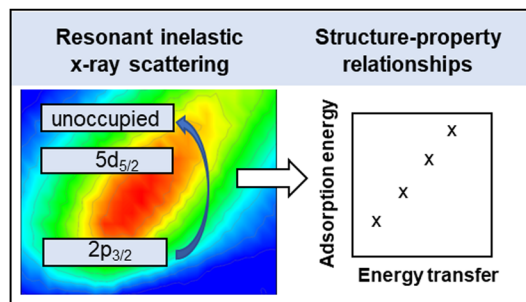
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### Conjugation-length dependence of regioregular oligo 3-alkyl(thienylene-vinylene)s demonstrates polyene-like behaviour with weak electron–electron correlations

Daniel W. Polak,\* Iain Andrews, George Farrow, Andrew J. Musser, Alex Auty, Dimitri Chekulaev, Julia A. Weinstein, Martin Heeney and Jenny Clark

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### Intermetallic alloy structure–activity descriptors derived from inelastic X-ray scattering

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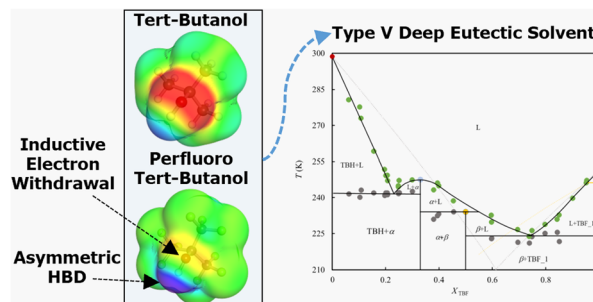


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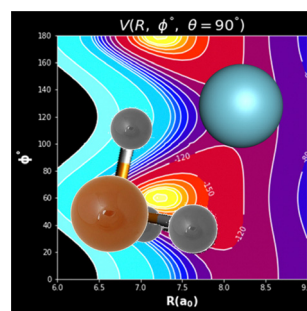
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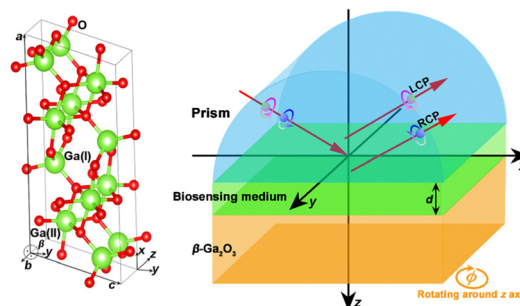
J. Salem,\* A. Badri, M. Salem, M. Mogren Al-Mogren and M. Hochlaf\*



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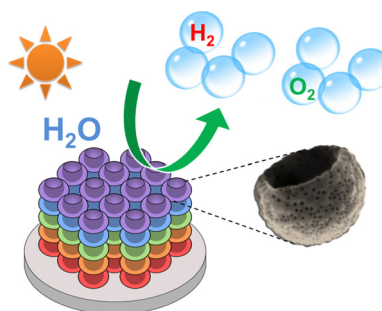
Guangyi Jia,\* Wenxuan Xue, Zhenxin Jia and Mathias Schubert\*



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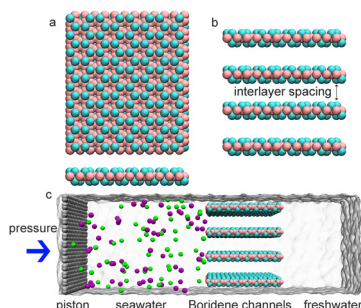
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Yuanxing Fang, Ronan Hodgson, Wei Cheat Lee, Huyen Le, Hon Wing Boaz Chan, Hassan M. Hassan, Ibrahim H. Alsohaimi, Giacomo E. Canciani, Rong Qian and Qiao Chen\*



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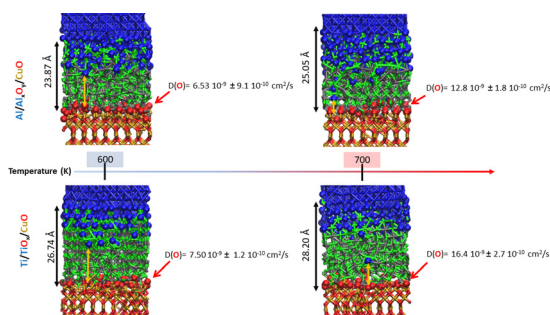
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## Efficient seawater desalination in lamellar nanochannel-based boridene filtration membrane

Shuxin He and Zonglin Gu\*

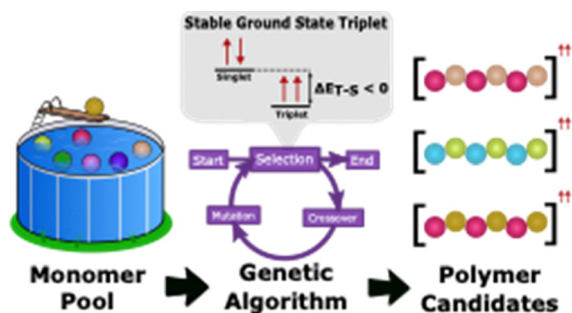
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## Initial stage of titanium oxidation in Ti/CuO thermites: a molecular dynamics study using ReaxFF forcefields

Hicham Jabraoui, Alain Estève, Sungwook Hong and Carole Rossi\*

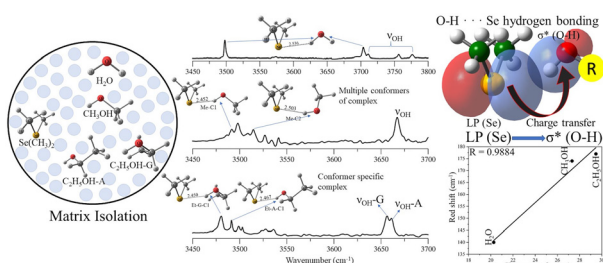
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## Using genetic algorithms to discover novel ground-state triplet conjugated polymers

Omri D. Abarbanel and Geoffrey R. Hutchison\*

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Hydrogen bond properties of Se in  $[\text{ROH-Se}(\text{CH}_3)_2]$  complexes (R = H,  $\text{CH}_3$ ,  $\text{C}_2\text{H}_5$ ): matrix-isolation infrared spectroscopy and theoretical calculations

Dhritabrata Pal, Sumit Kumar Agrawal, Amrita Chakraborty and Shamik Chakraborty\*

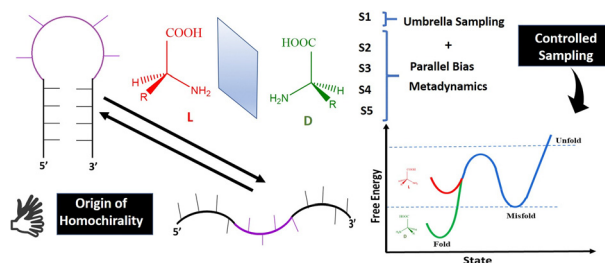


## RESEARCH PAPERS

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**Molecular insights into the stereospecificity of arginine in RNA tetraloop folding**

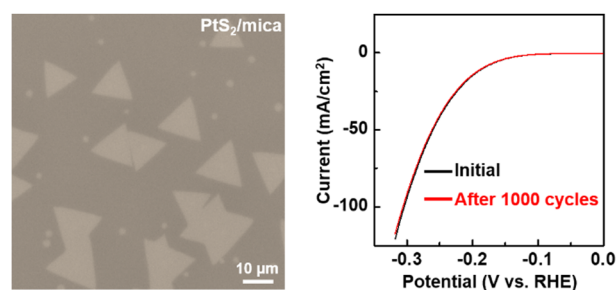
Amal Vijay and Arnab Mukherjee\*



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**Chemical vapor deposition of uniform bilayer PtS<sub>2</sub> flakes for electrocatalytic hydrogen evolution**

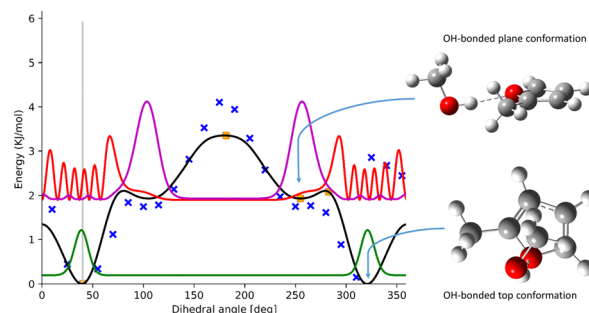
Yu-Qing Zhao, Liang Zhu, Bojian Zhou and Shaolong Jiang\*



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**Improved modeling of anharmonicity for furan microsolvation**

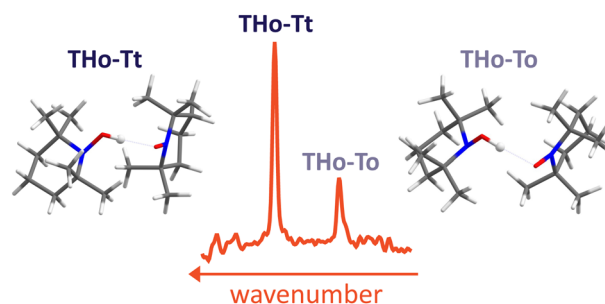
Wassja A. Kopp,\* Matthias L. Mödden,\* Narasimhan Viswanathan, Gabriel Rath\* and Kai Leonhard



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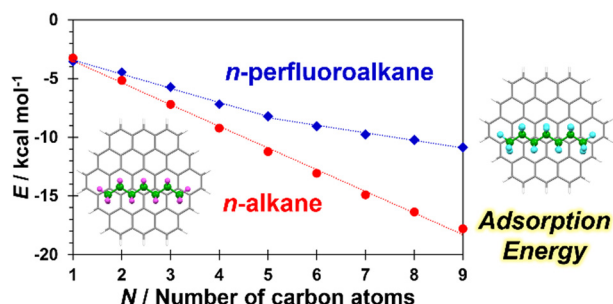
**Hydrogen sharing between two nitroxyl radicals in the gas phase and other microsolvation effects on the infrared spectrum of a bulky hydroxylamine**

Tajja L. Fischer, Martijn A. Tepaske and Martin A. Suhm\*



## RESEARCH PAPERS

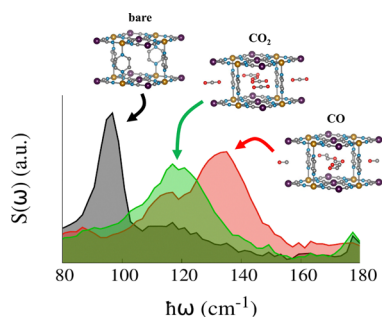
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### Analysis of intermolecular interactions of *n*-perfluoroalkanes with circumcoronene using dispersion-corrected DFT calculations: comparison with those of *n*-alkanes

Yoshihiro Kikkawa\* and Seiji Tsuzuki\*

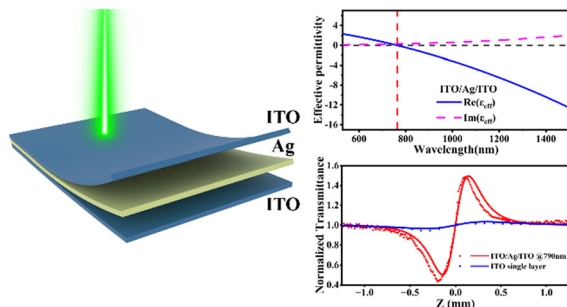
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### CO and CO<sub>2</sub> adsorption mechanism in Fe(pz)[Pt(CN)<sub>4</sub>] probed by neutron scattering and density-functional theory calculations

Ángel Fernández-Blanco, Lucía Piñeiro-López, Mónica Jiménez-Ruiz, Stephane Rols, José Antonio Real, Jose Sanchez Costa, Roberta Poloni\* and J. Alberto Rodríguez-Velamazán\*

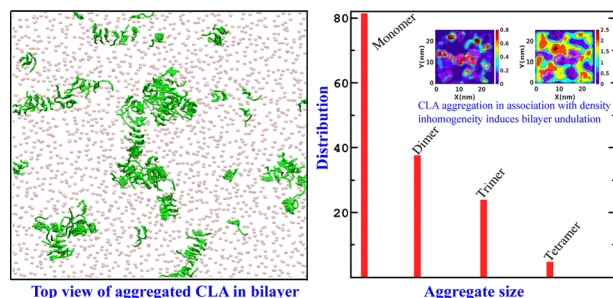
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### Boosting optical nonlinearity in epsilon-near-zero trilayer coatings

Zhida Guo, Dong Wu, Feilian Zhang, Jiannan Dong, Xiaofang Jiang,\* Peng Han and Yihang Chen\*

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### Aggregation of chlorophylls on plant thylakoid membranes using coarse-grained simulations

Renu Saini, Suleman Jalilahmad Ansari and Ananya Debnath\*

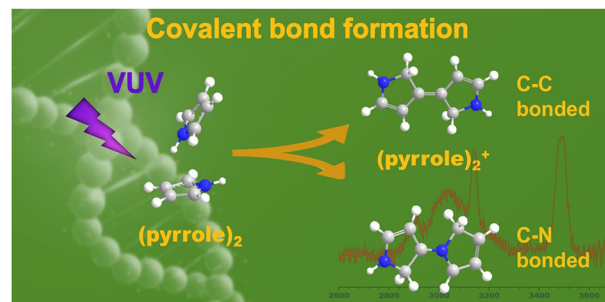


## RESEARCH PAPERS

11368

## Single-photon ionization induced C–C or C–N bond formation in pyrrole clusters

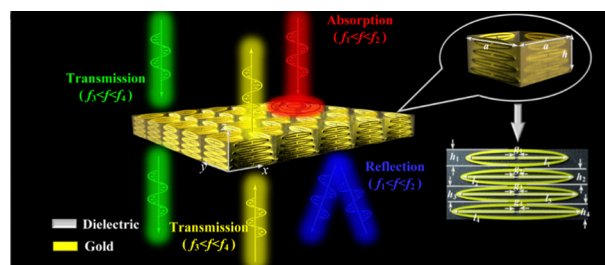
Chengcheng Wei, Xujian Chen, Yi Wang, Yujian Li, Jiao Gao, Min Xie\* and Yongjun Hu\*



11375

## Anapole-excited terahertz multifunctional spoof surface plasmon polariton directional Janus metastructures

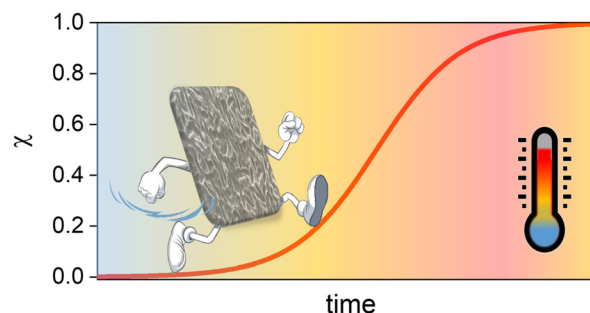
Hao Pan, Bing-xiang Li\* and Hai Feng Zhang\*



11387

## About determining reliable etching rates and the role of temperature in kinetic experiments on acidic wet chemical etching of silicon

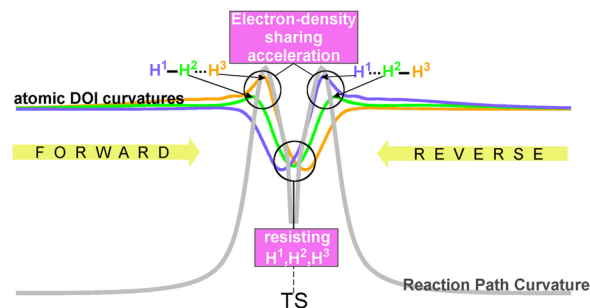
Anja Rietig,\* Thomas Langner and Jörg Acker



11398

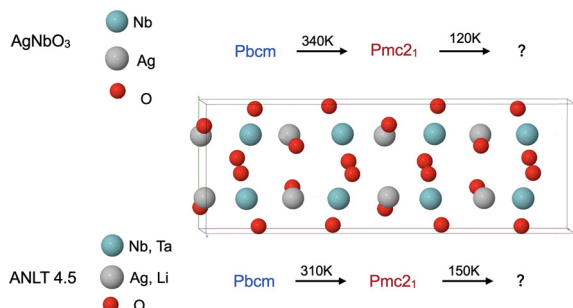
## New insight into atomic-level interpretation of interactions in molecules and reacting systems

Corentin Lefebvre, Hassan Khartabil and Eric Hénon\*



## RESEARCH PAPERS

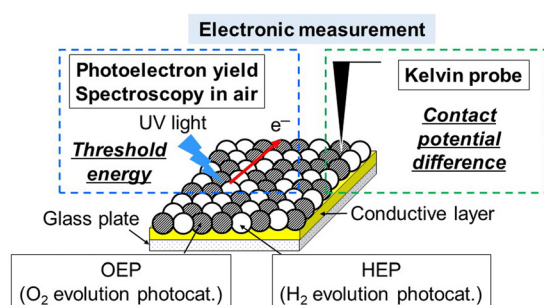
11410



### Temperature phase transitions in silver niobate and lithium tantalate-modified silver niobate ceramics

Alexander S. Krylov, Svetlana N. Krylova,\*  
Alexander N. Vtyurin, Eugene M. Roginskii,  
Li Jin, Ye Tian and Xiaoyong Wei

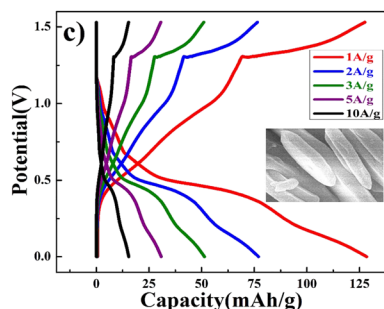
11418



### Examination of photocatalytic Z-scheme system for overall water splitting with its electronic structure

Tadaaki Tani,\* Yuichi Yamaguchi, Taisei Nishimi,  
Takayuki Uchida and Akihiko Kudo

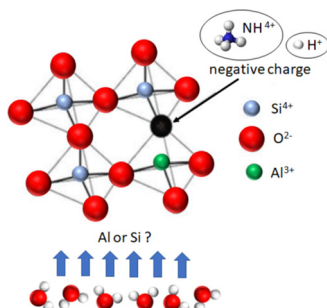
11429



### Framework structured $\text{Ce}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$ as a pseudocapacitive electrode of a hybrid (asymmetric) supercapacitor (HSC) for large scale energy storage applications

Mahatim Singh, Rakesh Mondal, Preetam Singh\* and  
Neeraj Sharma\*

11442



### Significance of the surface silica/alumina ratio and surface termination on the immersion freezing of ZSM-5 zeolites

Katherine E. Marak, Lucy Nandy, Divya Jain and  
Miriam Arak Freedman\*

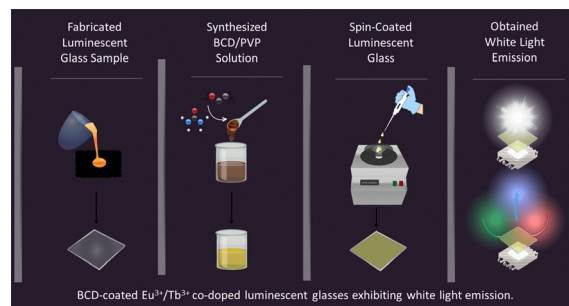


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11452

## The coupling of blue emitting carbon dots with $\text{Eu}^{3+}/\text{Tb}^{3+}$ co-doped luminescent glasses for utilization in white light emitting diodes

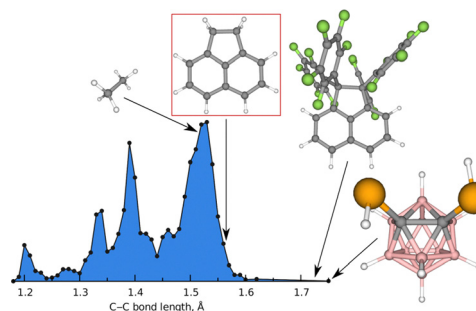
Ulaş Korkmaz, Beyza Özlem, Erdiñç Erol,  
Melis Özge Alas, Rükan Genç Altürk,  
Miray Çelikkilek Ersundu\* and Ali Erçin Ersundu\*



11464

## Accurate single crystal and gas-phase molecular structures of acenaphthene: a starting point in the search for the longest C–C bond

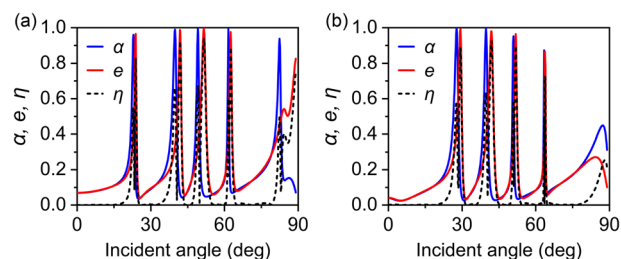
Yury V. Vishnevskiy,\* Arseniy A. Otyotov,  
Jan-Hendrik Lamm, Hans-Georg Stammer,  
Georgiy V. Girichev and Norbert W. Mitzel\*



11477

## A multi-band nonreciprocal thermal emitter involving a Weyl semimetal with a Thue–Morse multilayer

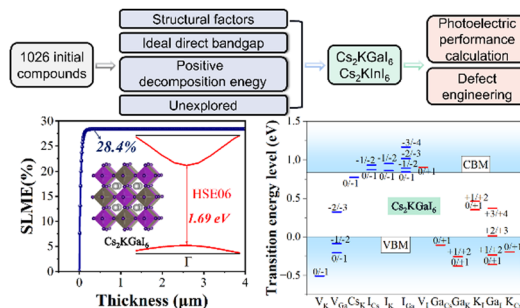
Jun Wu\* and Ye Ming Qing\*



11484

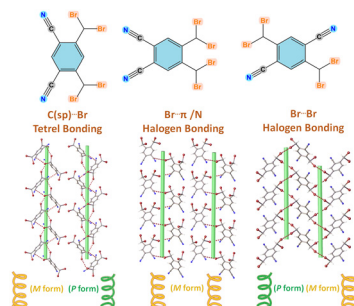
## Optoelectronic performance of perovskite $\text{Cs}_2\text{KMI}_6$ ( $\text{M} = \text{Ga}, \text{In}$ ) based on high-throughput screening and first-principles calculations

Fangfang Qi, Xin Lv, Jinhui Song, Xifeng Fu, Lingyi Meng\*  
and Can-Zhong Lu\*



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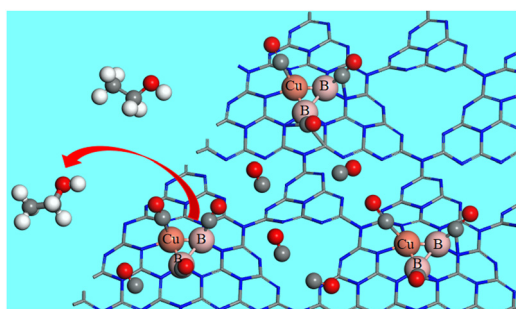
11493



### Engineering supramolecular helical assemblies via interplay between carbon(sp) tetrel and halogen bonding interactions

Burcu Dedeoglu, Ayşe Gül Gürek, Yunus Zorlu\* and Mehmet Menaf Ayhan\*

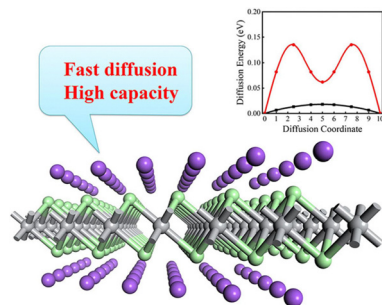
11501



### Immobilized triatomic CuB<sub>2</sub> clusters on 2D carbon nitride: highly selective conversion of CO to ethanol at low potentials

Zhichao Hao, Li-Juan Ma,\* Yaguang Guo, Jianfeng Jia and Hai-Shun Wu

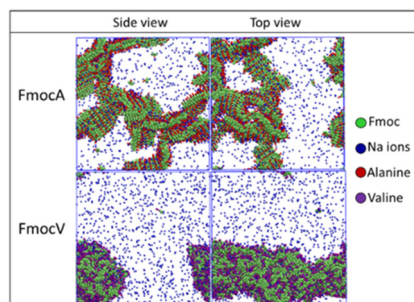
11513



### Two-dimensional TiCl<sub>2</sub>: a high-performance anode material for Na-ion batteries with high capacity and fast diffusion

Hong-Yao Zhu, Xiao-Juan Ye, Lan Meng, Xiao-Hong Zheng, Ran Jia and Chun-Sheng Liu\*

11522



### Solvent-controlled self-assembly of Fmoc protected aliphatic amino acids

Bharti Koshti, Hamish W A Swanson, Basil Wilson, Vivekshinh Kshtriya, Soumick Naskar, Hanuman Narode, King Hang Aaron Lau, Tell Tuttle\* and Nidhi Gour\*

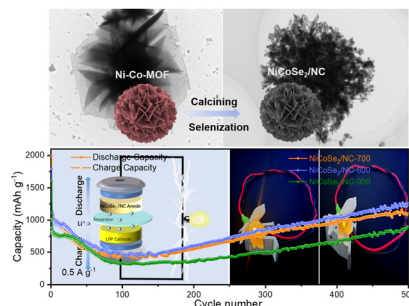


## RESEARCH PAPERS

11530

### Nitrogen-doped carbon decorated 3D NiCoSe<sub>2</sub> micro-flowers as high-performance anode materials for lithium-ion batteries

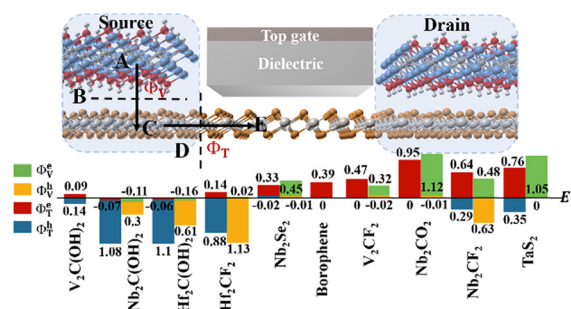
Jing Xu, Lingling Xie,\* Yu Niu, Honghua Chen, Yuhang Zhang, Yubin Jiang, Qing Han, Xuejing Qiu, Yongxia Miao, Limin Zhu\* and Xiaoyu Cao\*



11545

### Interfacial electronic properties between PtSe<sub>2</sub> and 2D metal electrodes: a first-principles simulation

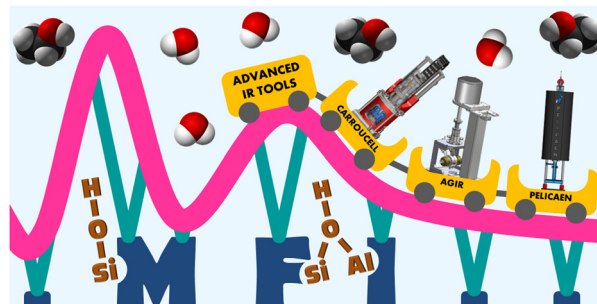
Xinyue Tian, Wenfei Zhang, Guang-Ping Zhang, Zong-Liang Li, Chuan-Kui Wang\* and Minglang Wang\*



11555

### Impact of the Si/Al ratio on the ethanol/water coadsorption on MFI zeolites revealed using original quantitative IR approaches

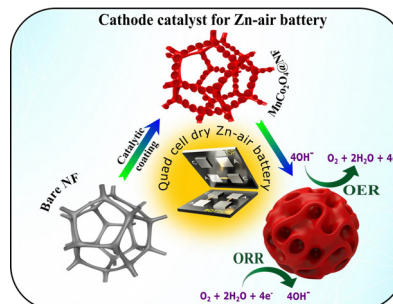
Rita Zakhia Douaihy, Louwanda Lakiss, Mohamad El-Roz, Yoann Levaque, Alexandre Vimont and Philippe Bazin\*



11566

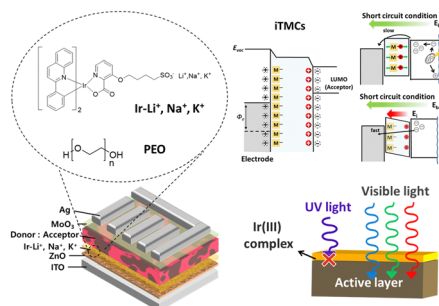
### Manganese–cobalt oxide as an effective bifunctional cathode for rechargeable Zn–air batteries with a compact quad-cell battery design

Khaleel Ahmed J. Dilshad and M. K. Rabinal\*



## RESEARCH PAPERS

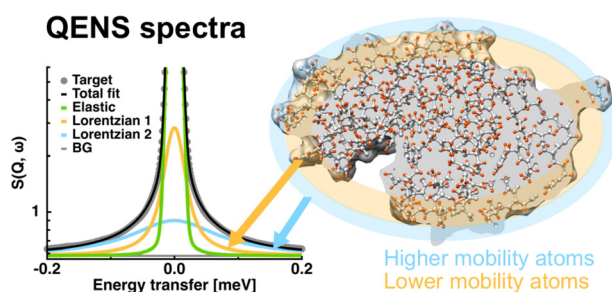
11577



### Ionic Ir(III) complex-interfacial layer for efficient carrier collection *via* induced electric dipole

Minsoo Lee, Hyun-Tak Kim, Ji Hoon Seo, Hyeon Oh Shin, Febrian Tri Adhi Wibowo, Sung-Yeon Jang,\* Kwanyong Seo\* and Tae-Hyuk Kwon\*

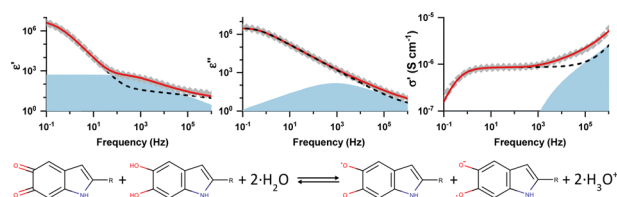
11586



### An improved analytical model of protein dynamics at the sub-nanosecond timescale

Tatsuhito Matsuo

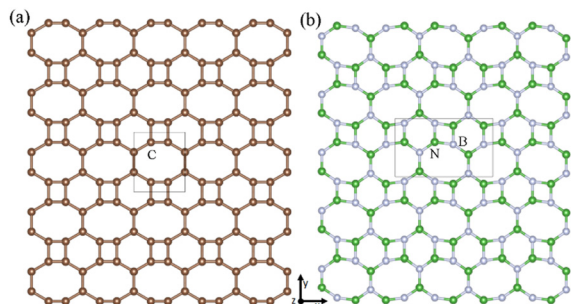
11601



### The influence of copper ions on the transport and relaxation properties of hydrated eumelanin

Pavel A. Abramov, Sergey S. Zhukov, Maxim Savinov, A. Bernardus Mostert and Konstantin A. Motovilov\*

11613



### DFT characterization of a new possible two-dimensional BN allotrope with a biphenylene network structure

Yang Han,\* Tingxiang Hu, Xiaochuang Liu, Shijie Jia, Hangbing Liu, Junyu Hu, Guolei Zhang, Longbin Yang, Guo Hong and Yi-Tung Chen

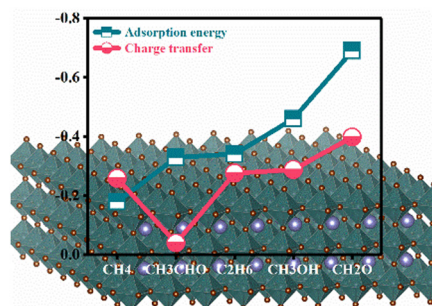


## RESEARCH PAPERS

11620

**All-inorganic halide perovskite CsPbBr<sub>3</sub>: a DFT study of a self-powered formaldehyde sensor**

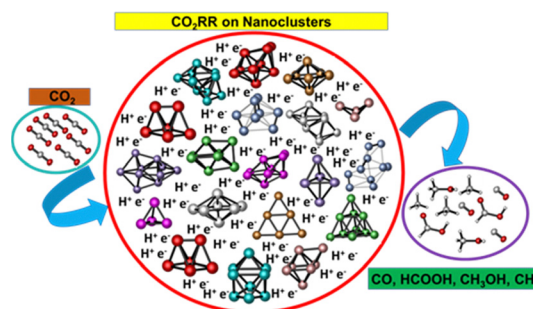
Xiaodong Liu, Jian Qiu, Qing Huang, Xianping Chen, Jiabing Yu\* and Jiading Bao\*



11630

**Electrocatalytic reduction of CO<sub>2</sub> on size-selected nanoclusters of first-row transition metal nanoclusters: a comprehensive mechanistic investigation**

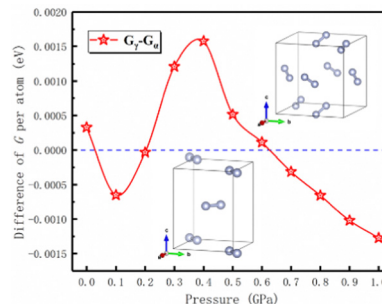
Rajesh Kumar Raju,\* Paramaconi Rodriguez and Edward N. Brothers



11653

**A simulation study on the phase transition behavior of solid nitrogen under extreme conditions**

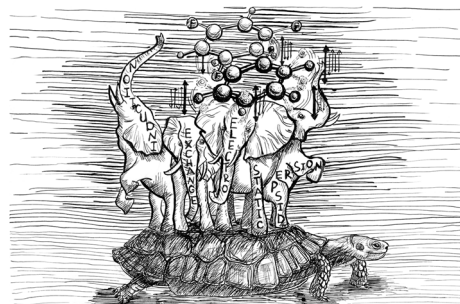
Han Qin, Sheng-Hai Zhu,\* Zhen Jiao, Fu-Sheng Liu, Zheng-Tang Liu and Qi-Jun Liu\*



11658

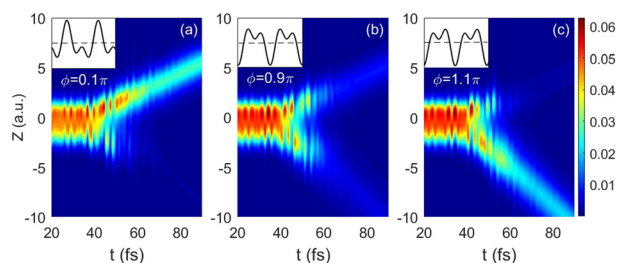
**A new computational tool for interpreting the infrared spectra of molecular complexes**

Alex Iglesias-Reguant, Heribert Reis, Miroslav Medveď, Josep M. Luis\* and Robert Zaleśny\*



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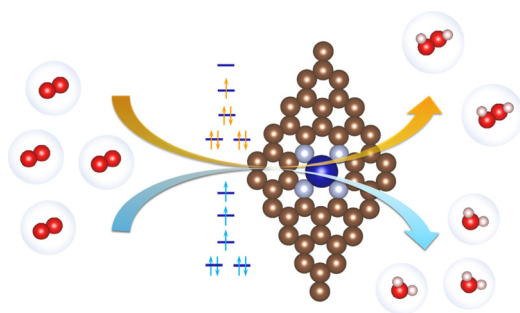
11665



### Controlling strong-field fragments of $\text{HD}^+$ with a synthesized two-color laser pulse

Hongbin Yao, Changhong Cao,\* Zhaopeng Sun, Wenliang Li, Yanhui Tao, Xiaohong Dong and Tuerdi Wumaier

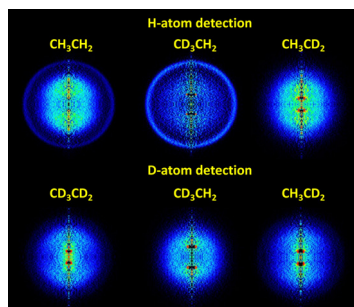
11673



### Correlation of the spin state and catalytic property of $\text{M-N}_4$ single-atom catalysts in oxygen reduction reactions

Wei Zhang, Jin-kong Pan, Yi-fan Yu, Xian-jie Zhang, Jia-hao Wang, Wen-xian Chen and Gui-lin Zhuang\*

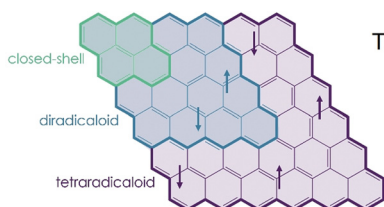
11684



### Imaging the photodissociation dynamics of internally excited ethyl radicals from high Rydberg states

Luis Rubio-Lago, David V. Chicharro, Sonia Marggi Poullain, Alexandre Zanchet, Greta Koumarianou, Pavle Glodic, Peter C. Samartzis, Alberto García-Vela and Luis Bañares\*

11697



Transition from closed- to open-shell electronic states:  
RAS-SF / RAS-srDFT  
(FT-)DFT

### Electronic structure of rhombus-shaped nanographenes: system size evolution from closed- to open-shell ground states

M. E. Sandoval-Salinas, R. Bernabeu-Cabañero, A. J. Pérez-Jiménez, E. San-Fabián and J. C. Sancho-García\*

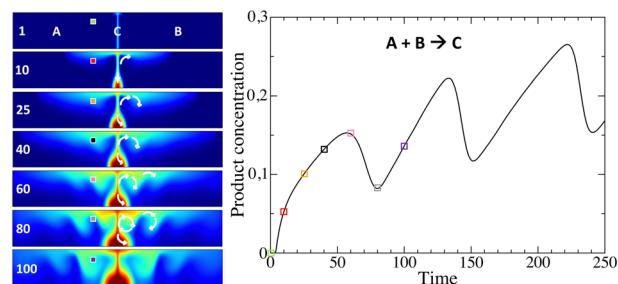


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11707

**Marangoni- vs. buoyancy-driven flows: competition for spatio-temporal oscillations in  $A + B \rightarrow C$  systems**

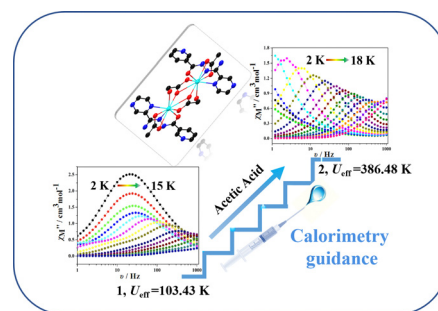
Adam Bigaj,\* Marcello A. Budroni,\* Dario Martín Escala and Laurence Rongy\*



11717

**Influence of lattice water molecules on the magnetization dynamics of binuclear dysprosium(III) compounds: insights from magnetic and *ab initio* calculations**

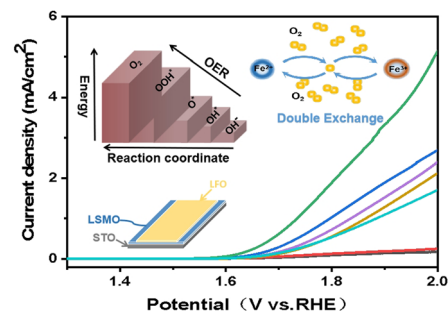
Jiyuan Du, Shilong Wei, Zhijie Jiang, Hongshan Ke, Lin Sun,\* Yiquan Zhang\* and Sanping Chen\*



11725

**The modulated oxygen evolution reaction performance of  $\text{LaFeO}_3$  with abundant electronic structures *via* a design of stoichiometry offset**

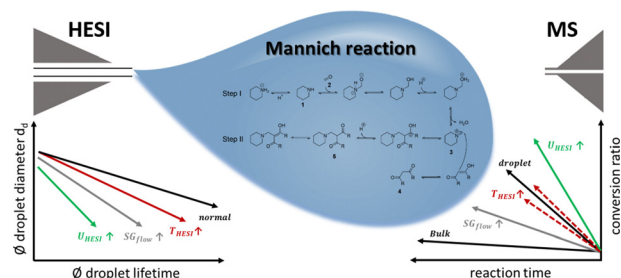
Yuan Zhang, Hang Xu, Mei Liu,\* Ji Qi, Linglong Hu, Ming Feng\* and Weiming Lü\*



11732

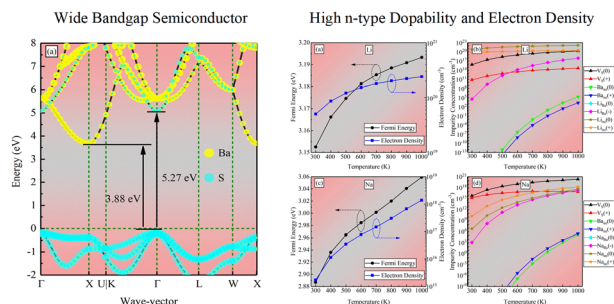
**Complex reaction kinetics of a Mannich reaction in droplets under electrospray conditions**

Martin Zühlke,\* Justin Koenig, Chris Prüfert, Stephan Sass, Toralf Beitz, Hans-Gerd Löhmannsröben, Christian Thoben, Stefan Zimmermann, Raphael D. Urban and Bernd Abel



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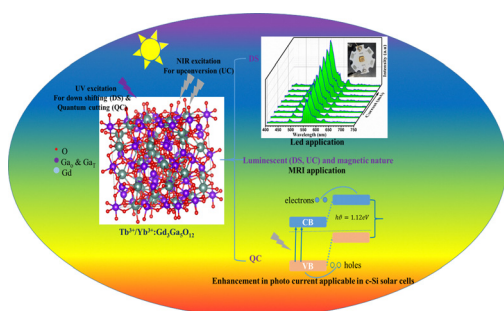
11745



## Theoretical insights into the defect performance of the wide bandgap semiconductor BaS

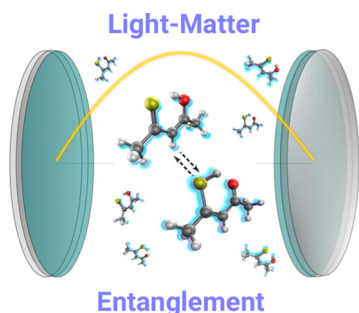
Yu Chen, S. W. Fan\* and G. Y. Gao

11756

Probing multimodal light emission from Tb<sup>3+</sup>/Yb<sup>3+</sup>-doped garnet nanophosphors for lighting applications

Neeraj Kumar Mishra, Kumar Shwetabh, Uttam K. Gautam and Kaushal Kumar\*

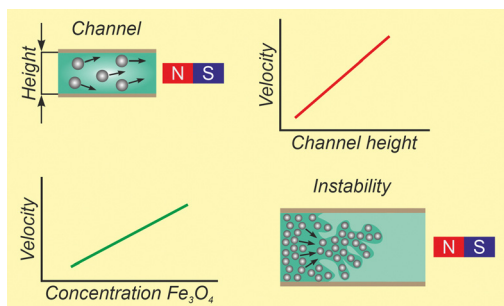
11771



## Cavity-catalyzed hydrogen transfer dynamics in an entangled molecular ensemble under vibrational strong coupling

Eric W. Fischer\* and Peter Saalfrank

11780



## Pattern formation and collective effects during the process of the motion of magnetic nanomotors in narrow channels

Boris Kichatov,\* Alexey Korshunov, Vladimir Sudakov, Vladimir Gubernov, Alexandr Golubkov, Alexey Kiverin, Alena Nastulyavichus and Sergey Kudryashov

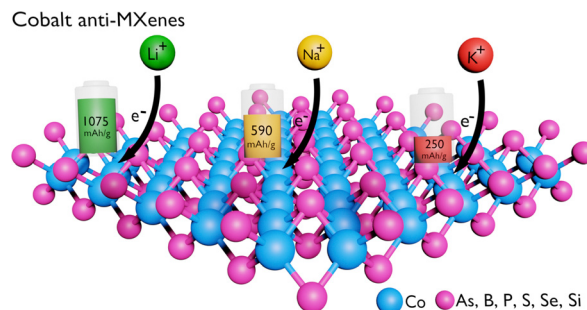


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11789

**Promising anode materials for alkali metal ion batteries: a case study on cobalt anti-MXenes**

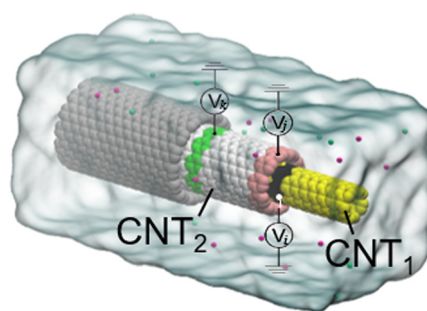
Subhadeep Banerjee, Ankita Narwal, Sandeep K Reddy and Sharma S. R. K. C. Yamijala\*



11805

**A controllable nanoscale telescopic arm designed by encoding the nested multi-walled carbon nanotubes**

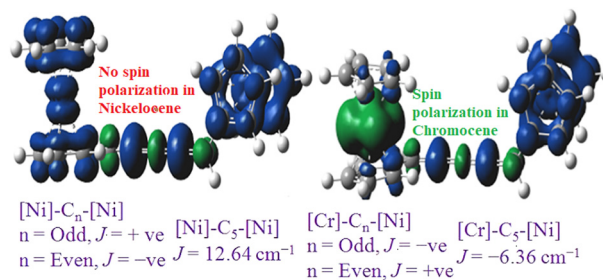
Wei Si,\* Liwei Wang, Xiaojing Lin, Gensheng Wu, Yin Zhang and Jingjie Sha\*



11816

**Metallocene-coupled cumulenes: a quest for chiral single-molecule magnets**

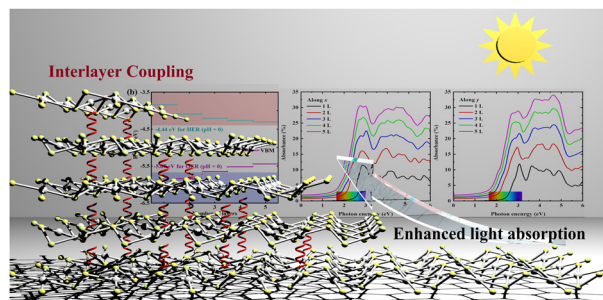
Soumik Das, Anirban Misra\* and Suranjan Shil\*



11827

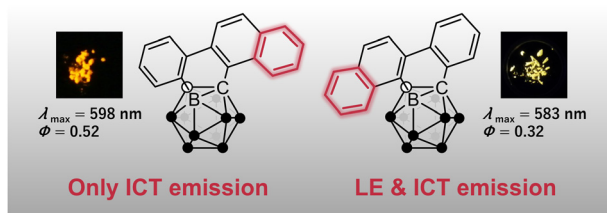
**Layer-dependent electronic structures and optical properties of two-dimensional PdSSe**

Feng Xiao, Wen Lei, Wei Wang, Yiping Ma, Xujia Gong and Xing Ming\*



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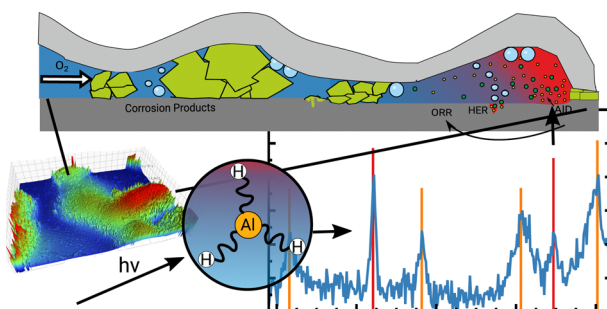
11839



### Tuning of the height of energy barrier between locally-excited and charge transfer states by altering the fusing position of *o*-carborane in phenylanthracene

Junki Ochi, Takumi Yanagihara, Kazuo Tanaka\* and Yoshiaki Chujo

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### Role of aluminium hydrides in localised corrosion of aluminium revealed by *operando* Raman spectroscopy

Erlind Mysliu, Otto Lunder and Andreas Erbe\*

