

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(15) 10189–11002 (2023)



## Cover

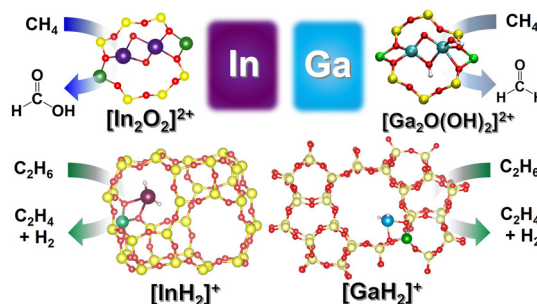
See Marta Pineiro *et al.*,  
pp. 10263–10277.  
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*Phys. Chem. Chem. Phys.*,  
2023, 25, 10263.

## PERSPECTIVES

## 10211

### In- and Ga-oxo clusters/hydrides in zeolites: speciation and catalysis for light-alkane activations/transformations

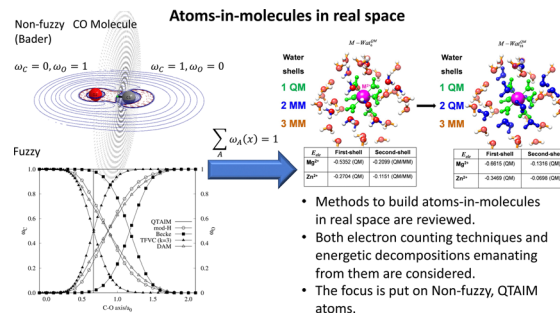
Huang Mengwen, Shinsaku Yasumura, Takashi Toyao, Ken-ichi Shimizu and Zen Maeno\*



## 10231

### Atoms in molecules in real space: a fertile field for chemical bonding

Ángel Martín Pendás,\* Evelio Francisco, Dimas Suárez, Aurora Costales, Natalia Díaz, Julen Munárriz, Tomás Rocha-Rinza and José Manuel Guevara-Vela



- Methods to build atoms-in-molecules in real space are reviewed.
- Both electron counting techniques and energetic decompositions emanating from them are considered.
- The focus is put on Non-fuzzy, QTAIM atoms.



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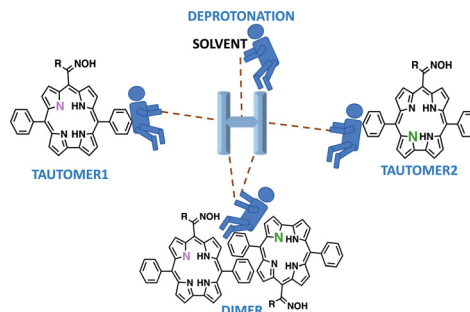


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## The role of solvents and concentrations in the properties of oxime bearing A<sub>2</sub>B corroles

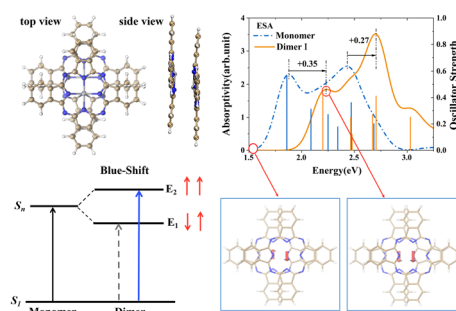
Ana Clara B. Rodrigues, Susana M. M. Lopes, Carla Cunha, João Braz, Teresa M. V. D. Pinho e Melo, J. Sérgio Seixas de Melo and Marta Pineiro\*



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## Effects of aggregation on the structures and excited-state absorption for zinc phthalocyanine

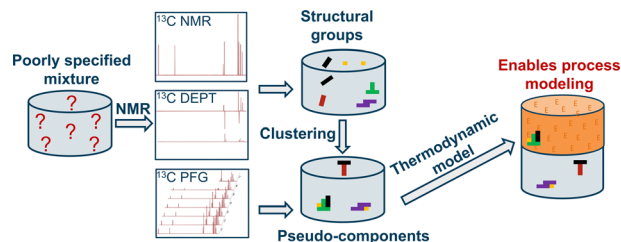
Hongjuan Zhu, Danyang Zhang, Eryin Feng and Xiaowei Sheng\*



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## Rational method for defining and quantifying pseudo-components based on NMR spectroscopy

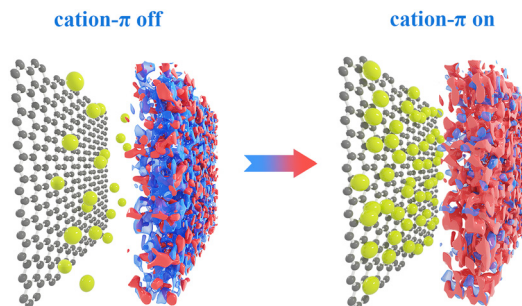
Thomas Specht, Kerstin Münnemann, Hans Hasse and Fabian Jirasek\*



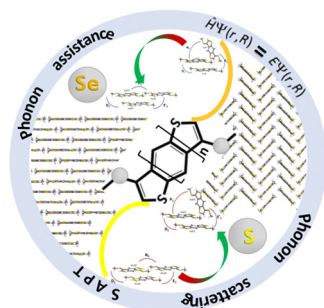
10301

## The evolution of anionic nanoclusters at the electrode interface in water-in-salt electrolytes

Lei Zhang, Yuanxi Yu, Liumin Suo, Wei Zhuang, Lunhua He, Xiaohua Zhang,\* Liang Hong\* and Pan Tan\*



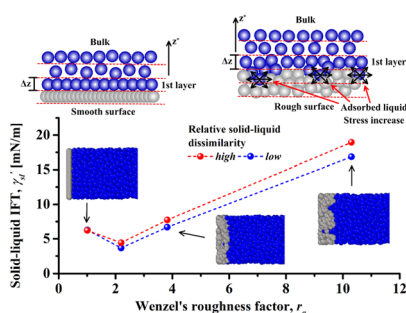
10313



### Theoretical study of the tuning role of $\beta$ -methylthio or $\beta$ -methylselenyl on the charge-transport properties of acenedithiophenes derivatives

Hui-Yuan Li, Gui-Ya Qin, Pan-Pan Lin, Xiao-Qi Sun, Jian-Xun Fan, Rui Wang, Hui Li, Lu-Yi Zou, Jing-Fu Guo and Ai-Min Ren\*

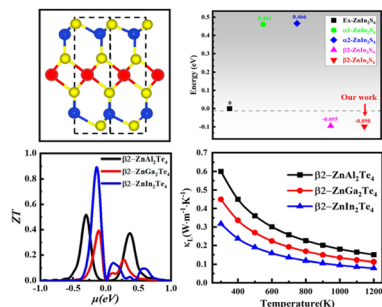
10325



### The effective interfacial tensions between pure liquids and rough solids: a coarse-grained simulation study

J. D. Hernández Velázquez,\* G. Sánchez-Balderas, A. Gama Goicochea and E. Pérez\*

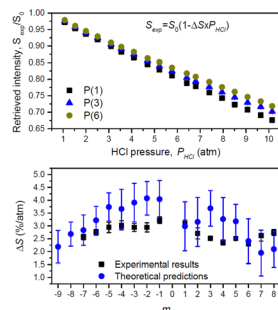
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### High mobility and excellent thermoelectric performance monolayer $\text{ZnX}_2\text{Z}_4$ ( $\text{X} = \text{In}, \text{Al}, \text{Ga}$ ; $\text{Z} = \text{S}, \text{Se}, \text{Te}$ ) materials

Li Shi, Chunyan Lv,\* Haoran Wei, Wangping Xu,\* Rui Wang, Jing Fan and Xiaozhi Wu\*

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### Pressure dependence of the measured line intensity and super-Lorentzian effects in the absorption spectra of pure HCl

Ha Tran,\* Gang Li, Ngoc Hoa Ngo and Volker Ebert



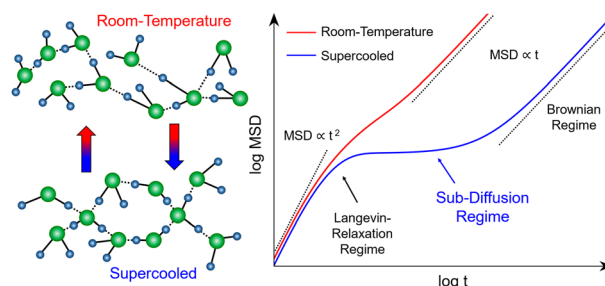


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### Topology induced crossover between Langevin, subdiffusion, and Brownian diffusion regimes in supercooled water

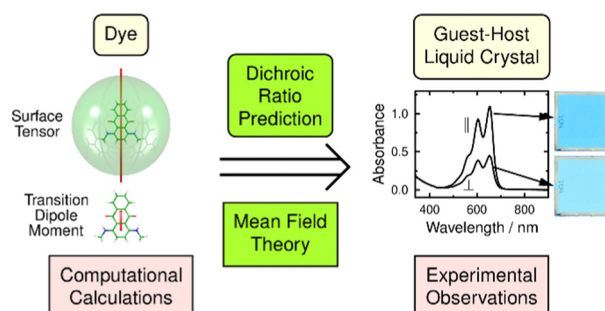
Kaicheng Zhu, Saber Naserifar,  
William A. Goddard III\* and Haibin Su\*



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### Dyes for guest–host liquid crystal applications: a general approach to the rapid computational assessment of useful molecular designs

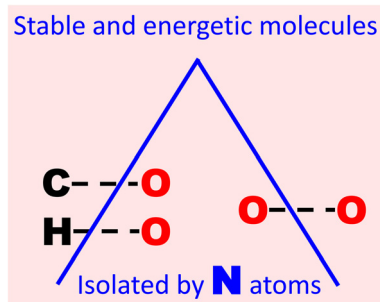
Mark T. Sims, Laurence C. Abbott, Richard J. Mandle,  
John W. Goodby and John N. Moore\*



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### Simple rule for linking atoms to construct high energy isomers

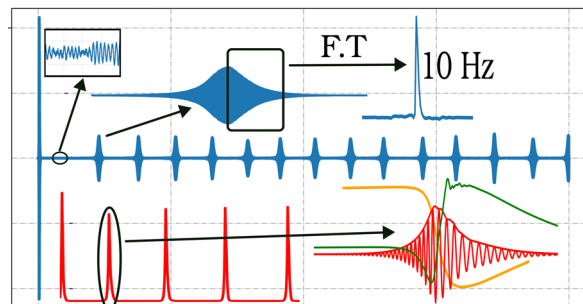
Rong Wang and Chaoyang Zhang\*



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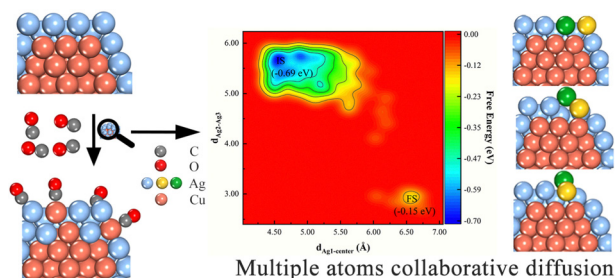
### Dipolar field effects in a solid-state NMR maser pumped by dynamic nuclear polarization

Vineeth Francis Thalakkottoor Jose Chacko and  
Daniel Abergel\*



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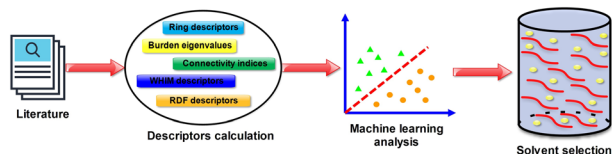
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### A collaborative diffusion mechanism of multiple atoms during Cu–Ag bimetal surface reconstruction

Xue Yan, Xiangxiang Wang, Jingli Han, Xiangjian Du, Zhongyi Liu and Yongpeng Yang\*

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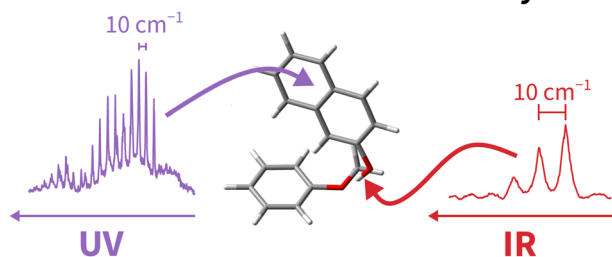


### Easy and fast prediction of green solvents for small molecule donor-based organic solar cells through machine learning

Asif Mahmood, Yahya Sandali and Jin-Liang Wang\*

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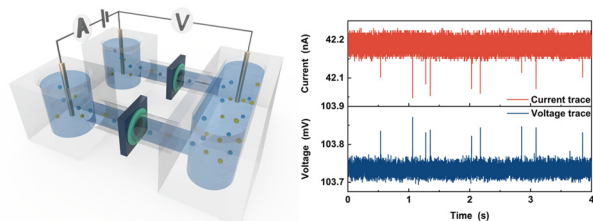
### Dual Franck-Condon activity



### Subtle hydrogen bond preference and dual Franck–Condon activity – the interesting pairing of 2-naphthol with anisole

Arman Nejad,\* Ariel F. Pérez Mellor, Manuel Lange, Ivan Alata, Anne Zehnacker and Martin A. Suhm

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### Detection of DNA translocations in a nanopore series circuit using a current clamp

Fei Zheng, Yi Tao, Wei Xu and Jingjie Sha\*

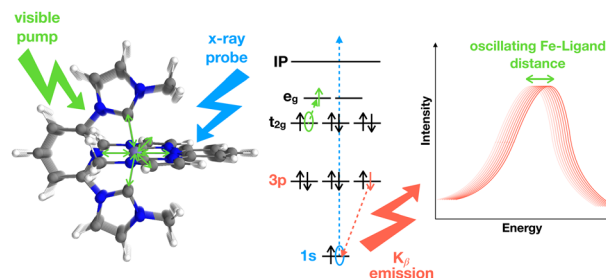


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**Sensitivity of K $\beta$  mainline X-ray emission to structural dynamics in iron photosensitizer**

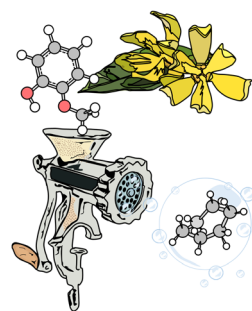
Johanna Rogvall, Roshan Singh, Morgane Vacher\* and Marcus Lundberg\*



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**DFT insights into competing mechanisms of guaiacol hydrodeoxygenation on a platinum cluster**

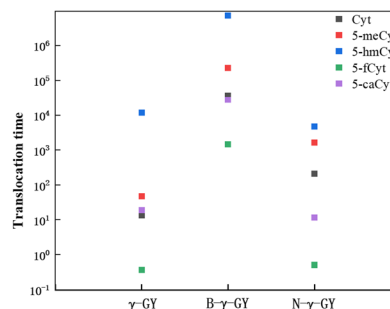
Chiara Nania, Marco Bertini, Laura Gueci, Francesco Ferrante\* and Dario Duca



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***Ab initio* studies on graphyne (GY) for the detection of rare bases in DNA**

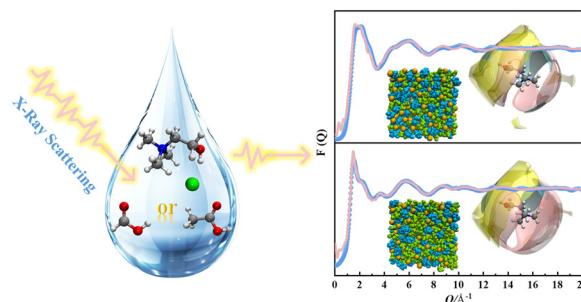
Mengdan Lv, Ruirui Li, Xia Zeng, Lingxia Jin,\* Caibin Zhao, Yanhong Gao, Min Jiang, Gongwei Qin, Chen Li and Shengrui Zhang\*



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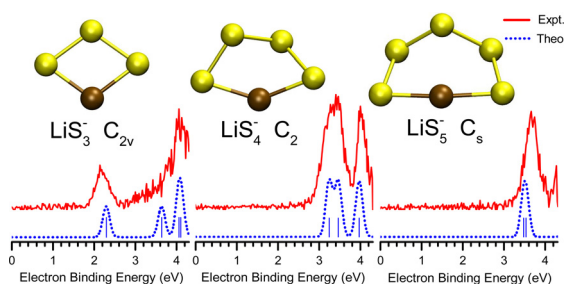
**Structure of choline chloride-carboxylic acid deep eutectic solvents by wide-angle X-ray scattering and DFT calculations**

Keke Chai, Yongquan Zhou,\* Xingmei Lu, Toshio Yamaguchi, Koji Ohara, Hongyan Liu and Fayan Zhu



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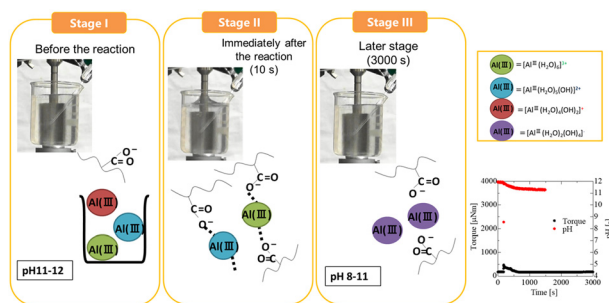
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### Structures and bonding properties of lithium polysulfide clusters $\text{LiS}_n^{-/0}$ ( $n = 3-5$ ) and $\text{Li}_2\text{S}_4^{-/0}$ : size-selected anion photoelectron spectroscopy and theoretical calculations

Zhen-Chao Long, Zhi-You Wei, Kai-Wen Liu, Xi-Long Li, Xi-Ling Xu, Hong-Guang Xu and Wei-Jun Zheng\*

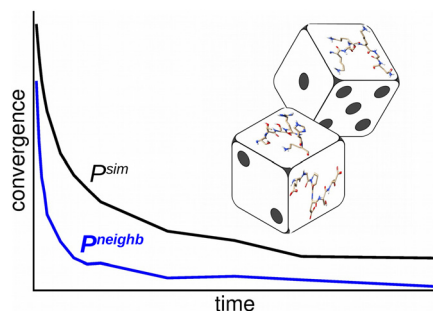
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### Unpredictable polymeric flow dynamics with reaction between HPAM and $\text{Al}^{3+}$ by comparison between pre- and post-reaction fluid properties

Sae Hirano, Yuichiro Nagatsu, Ryuta X. Suzuki and Jun Iijima\*

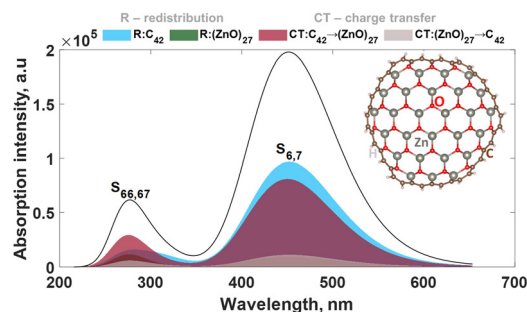
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### Description of conformational ensembles of disordered proteins by residue-local probabilities

Adolfo Bastida\*, José Zúñiga, Beatriz Miguel and Miguel A. Soler\*

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### Nature of photoexcited states in ZnO-embedded graphene quantum dots

Ivan Shtepliuk\* and Rositsa Yakimova

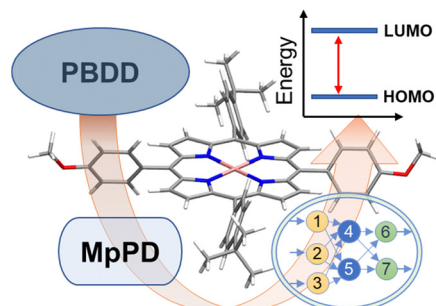


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# Deep transfer learning for predicting frontier orbital energies of organic materials using small data and its application to porphyrin photocatalysts

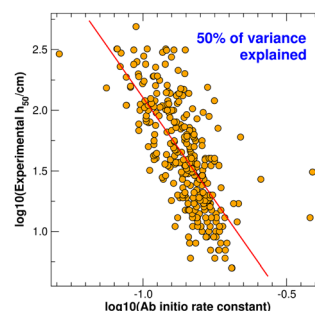
An Su,\* Xin Zhang, Chengwei Zhang, Debo Ding, Yun-Fang Yang, Keke Wang and Yuan-Bin She\*



10550

# Impact sensitivities of energetic materials derived from easy-to-compute *ab initio* rate constants

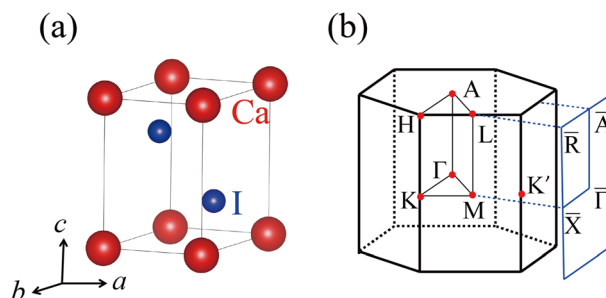
Romain Claveau, Julien Glorian and Didier Mathieu\*



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# Straight and twisted open nodal-line phonon states in the $\text{CaI}_2$ family of materials

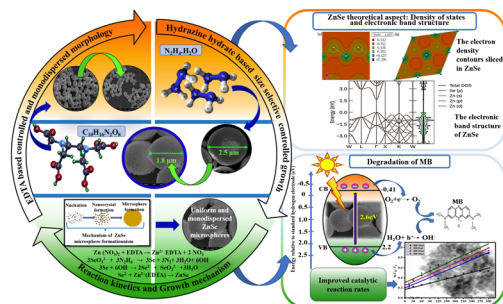
Meng-Xin Wu, Da-Shuai Ma,\* Tie Yang, Yu-Hao Wei, Ke Chai, Peng Wang, Biao Wang and Min-Quan Kuang\*



10567

# Controlled synthesis of monodispersed ZnSe microspheres for enhanced photo-catalytic application and its corroboration using density functional theory

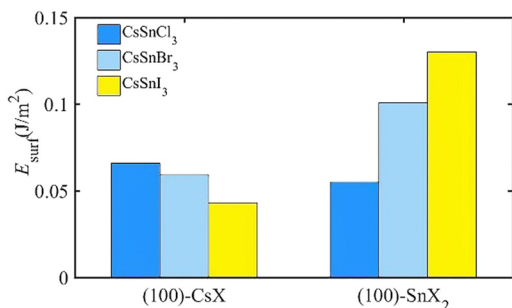
Prachi Chopade, Vikas Kashid, Niteen Jawale, Sunit Rane, Shweta Jagtap,\* Anjali Kshirsagar and Suresh Gosavi\*





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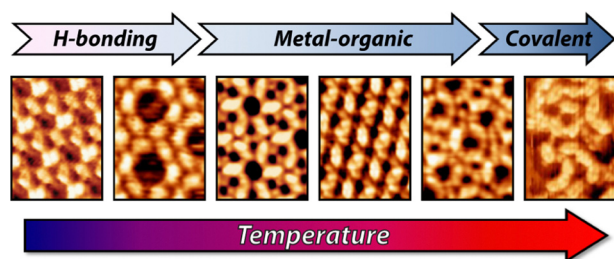
10583



### Surface energy and surface stability of cesium tin halide perovskites: a theoretical investigation

Yan-Jin Chen, Chunju Hou and Yi Yang\*

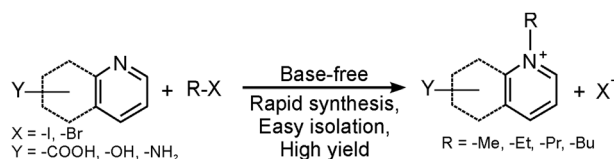
10591



### Self-assembly of *s*-indacene-tetrone on Cu(111): molecular trapping and patterning of Cu adatoms

Nataliya Kalashnyk, Adam Hassan Denawi, Frédéric Dumur, Didier Gigmes, Xavier Bouju\* and Sylvain Clair\*

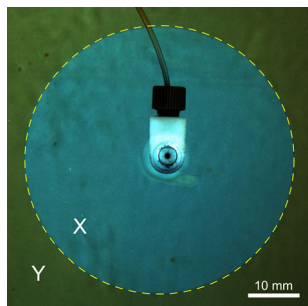
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### Ground-state intramolecular proton transfer inhibits the selective methylation on quinoline and pyridine derivatives

Supphachok Chanmungkalakul, Shiqing Huang, Xia Wu, Esther Cai Xia Ang, Zi-Qi Yang, Yongxin Li, Xiaoyu Yan, Choon-Hong Tan, Davin Tan\* and Xiaogang Liu\*

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### Effect of radial advection on autocatalytic reaction–diffusion fronts

Alessandro Comolli, L. Negrojević, Fabian Brau and A. De Wit\*

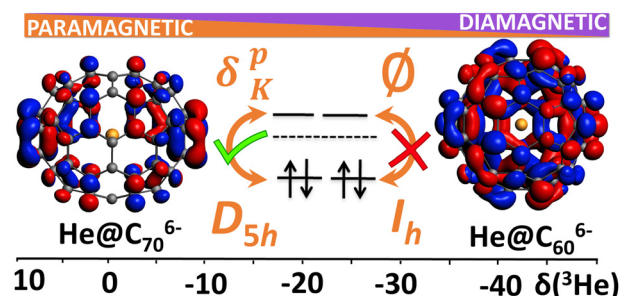


## RESEARCH PAPERS

10620

# The essential role of symmetry in understanding $^3\text{He}$ chemical shifts in endohedral helium fullerenes

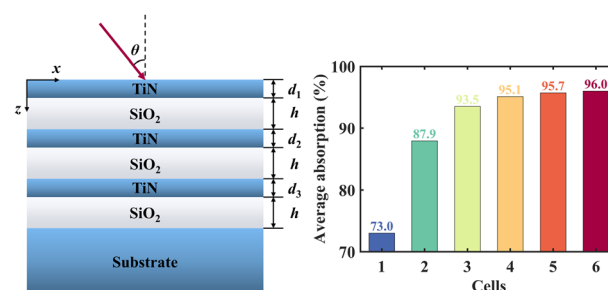
Jan Vicha,\* Juha Vaara\* and Michal Straka



10628

# Pattern-free solar absorber driven by superposed Fabry–Perot resonances

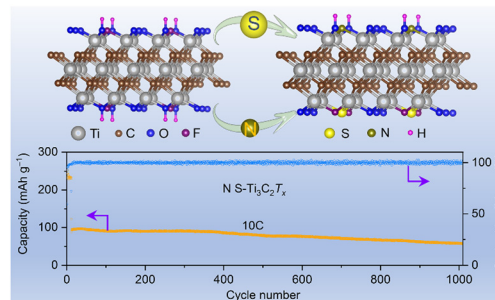
Haotuo Liu, Kun Yu, Kaihua Zhang, Qing Ai,\* Ming Xie and Xiaohu Wu\*



10635

# Nitrogen and sulfur co-doped $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes for high-rate lithium-ion batteries

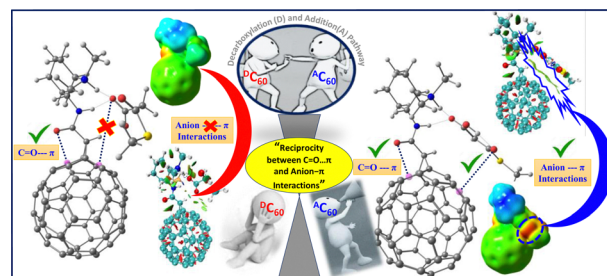
Renfei Cheng, Tao Hu, Jinxing Yang, Zuohua Wang, Weizhen Wang, Yan Liang, Zhiqing Yang, Hongwang Zhang and Xiaohui Wang\*



10647

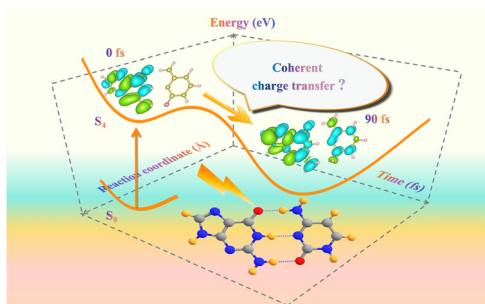
# Reciprocity of $\text{C}=\text{O} \cdots \pi$ interactions with the dominant anion– $\pi$ on fullerene ( $\text{C}_{60}$ )– amine-based organocatalysts: a mechanistic elucidation for addition vs. decarboxylation reaction

Murugesan Panneerselvam, Hiregange Akash and Archita Patnaik\*



## RESEARCH PAPERS

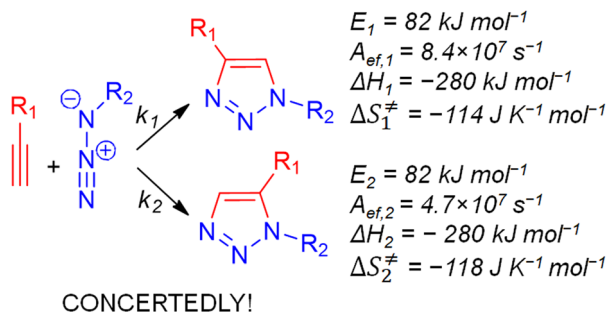
10661



### The dynamical temporal behaviors of guanine–cytosine coherent charge transfer

Lixia Zhu, Qiao Zhou, Yongfeng Wan, Qi Li, Yu Wan, Hang Yin and Ying Shi\*

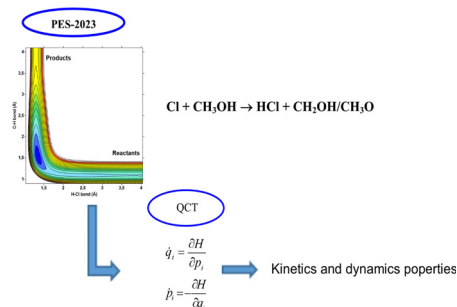
10671



### Probing kinetic and mechanistic features of bulk azide–alkyne cycloaddition

Andrey Galukhin,\* Roman Aleshin, Roman Nosov and Sergey Vyazovkin\*

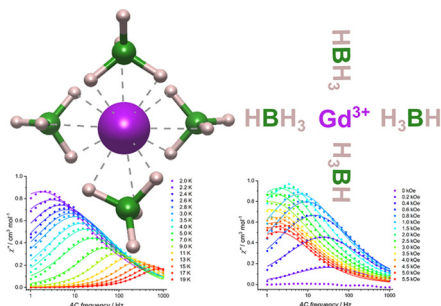
10678



### Kinetics and dynamics study of the Cl(<sup>2</sup>P) + CH<sub>3</sub>OH reaction based on an analytical potential energy surface

Cipriano Rangel and Joaquin Espinosa-Garcia\*

10689



### Approaching the free-ion limit in magnetically isotropic gadolinium(III) via borohydride ligands

Michał Magott\* and Wojciech Wegner\*

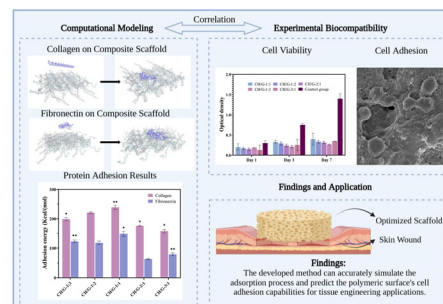


## RESEARCH PAPERS

10697

## Investigating the correlation between the protein adhesion simulation and the biocompatibility of polymeric substrate for skin-tissue-engineering applications

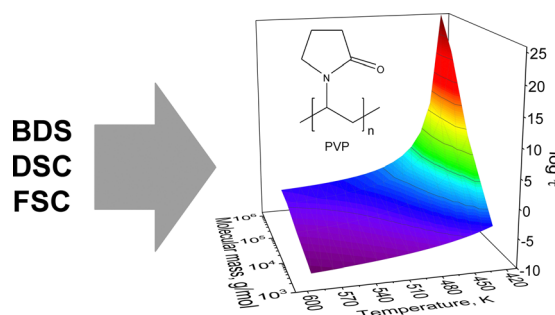
Saeed Seifi, Mohammad Ali Bakhtiari, Hossein Shaygani, Amir Shamloo\* and Aram Almasi-Jaf



10706

## Some aspects of the glass transition of polyvinylpyrrolidone depending on the molecular mass

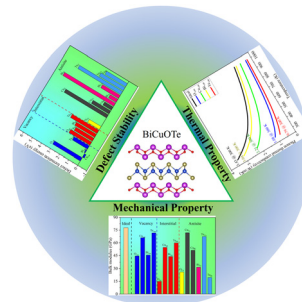
Semen Lapuk, Marina Ponomareva, Marat Ziganshin, Radik Larionov, Timur Mukhametzyanov, Christoph Schick, Ivan Lounev and Alexander Gerasimov\*



10715

## The effects of point defects on thermal-mechanical properties of BiCuOTe: a first-principles study

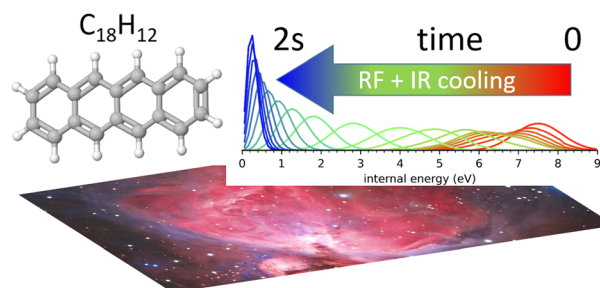
Ming Jiang, Xing-Can Guo, Xiao-Tao Zu\* and Chandra Veer Singh\*



10726

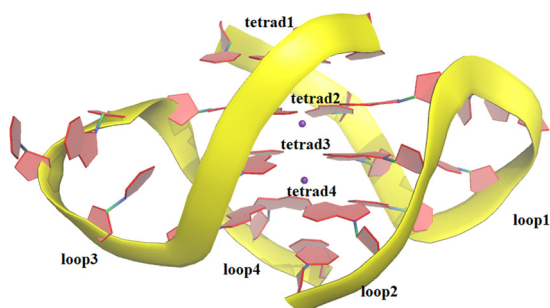
## Efficient radiative cooling of tetracene cations $C_{18}H_{12}^+$ : absolute recurrent fluorescence rates as a function of internal energy

Jérôme Bernard,\* MingChao Ji, Suvasthika Indrajith, Mark H. Stockett, José E. Navarro Navarrete, Naoko Kono, Henrik Cederquist, Serge Martin, Henning T. Schmidt and Henning Zettergren



## RESEARCH PAPERS

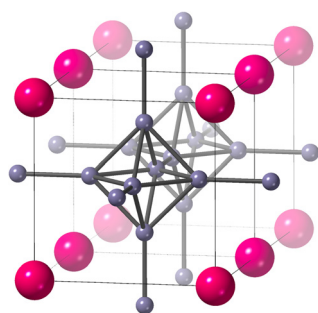
10741



### Binding of berberine derivatives to G-quadruplex: insight from a computational study

Mengxin Li, Yalong Cong, Yifei Qi\* and John Z. H. Zhang\*

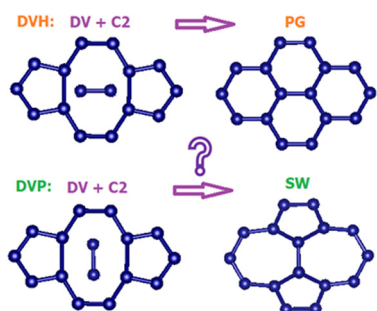
10749



### The contribution of phonons to the thermal expansion of some simple cubic hexaboride structures: $\text{SmB}_6$ , $\text{CaB}_6$ , $\text{SrB}_6$ and $\text{BaB}_6$

Li Li, Keith Refson and Martin T Dove\*

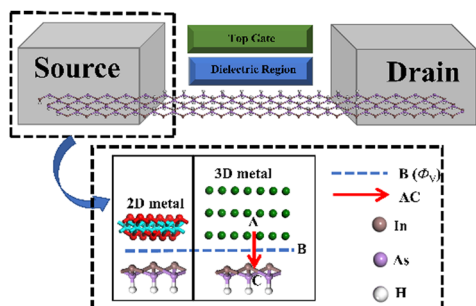
10759



### Healing double vacancy defects on graphene: reconstruction by $\text{C}_2$ adsorption

Parisa Alamdari, Farhad Sharif,\* Saeedeh Mazinani, German Sastre\* and Hermenegildo Garcia

10769



### Systematic investigation of the mechanical, electronic, and interfacial properties of high mobility monolayer InAs from first-principles calculations

Wenjing Yu, Jingzhen Li,\* Yi Wu, Jing Lu and Yongzhe Zhang\*



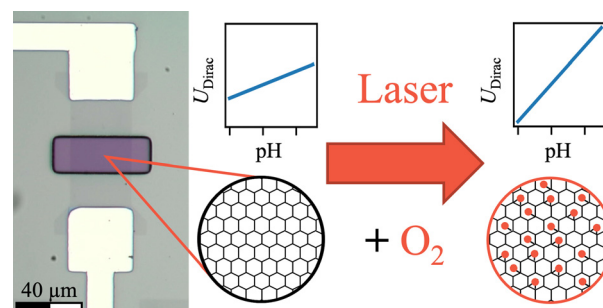


## RESEARCH PAPERS

10778

**Laser-induced tuning of graphene field-effect transistors for pH sensing**

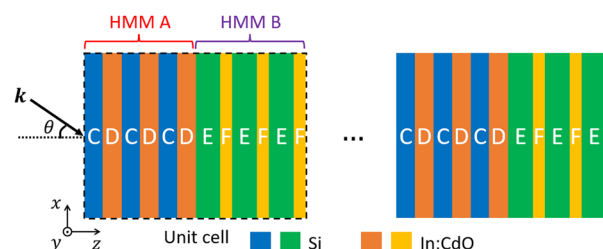
Aku Lampinen, Erich See, Aleksei Emelianov,  
Pasi Myllyperkiö, Andreas Johansson and  
Mika Pettersson\*



10785

**A redshifted photonic bandgap and wide-angle polarization selection in an all-hyperbolic-metamaterial one-dimensional photonic crystal**

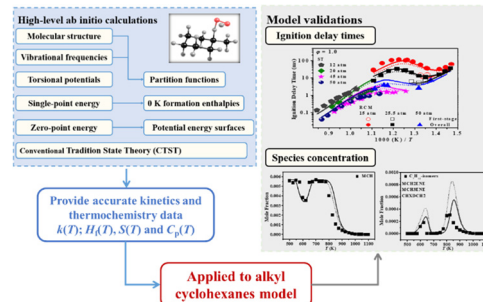
Feng Wu,\* Dejun Liu, Hongju Li and Mingku Feng



10795

**From electronic structure to model application for alkyl cyclohexane combustion chemistry: H-atom abstraction reactions by HO<sub>2</sub> radical**

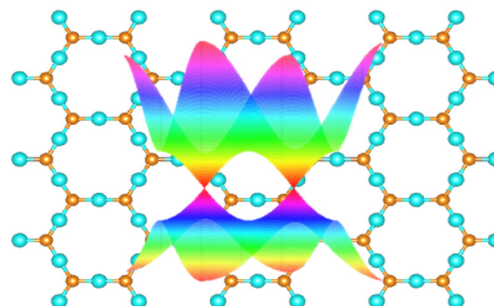
Mingxia Liu, Xin Hui, Xin Xue, Yuzhen Lin and  
Chong-Wen Zhou\*



10811

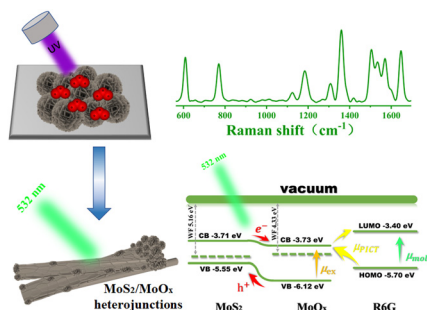
**A family of robust Dirac cone materials: two-dimensional hexagonal M<sub>3</sub>X<sub>2</sub> (M = Zn/Cd/Hg, X = Si/Ge)**

Qiuyang Li, Cuixia Yan,\* Chenchen Qi, Shi Qiu,  
Ting Yang and Jinming Cai



## RESEARCH PAPERS

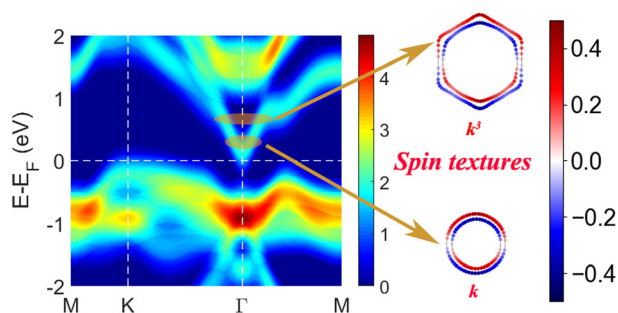
10820



### Ultraviolet-ozone concomitantly induced MoS<sub>2</sub>/MoO<sub>x</sub> heterostructures with improved SERS performance

Zhao Wei, Songyang Xie, Wei Xiong,\* Shuwen Zen, Dong Chen,\* Tao Jiang, Da Chen, Jun Zhou and Chenjie Gu\*

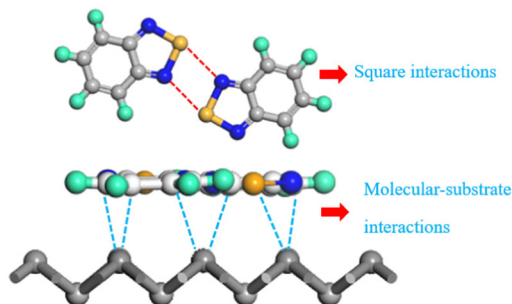
10827



### Hexagonal warping effect in the Janus group-VIA binary monolayers with large Rashba spin splitting and piezoelectricity

Shao-Bo Chen, San-Dong Guo, Wan-Jun Yan, Zhao-Yi Zeng,\* Mei Xu,\* Xiang-Rong Chen\* and Hua-Yun Geng

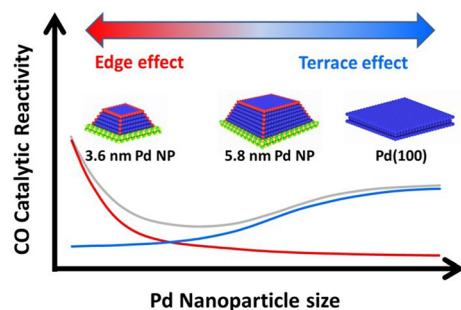
10836



### First-principles study of square chalcogen bond interactions and its adsorption behavior on silver surface

Hui Wang,\* Bin Li, Xiaoting Wang, Fu Yin, Qiaoyu Wei, Xudong Wang, Yuxiang Ni and Hongyan Wang

10845



### *In situ* study of catalytic CO oxidation on ultrathin MgO film supported Pd nanoparticles by sum frequency generation: size and site effects

Jijin Wang,\* Aimeric Ouvrard, Wanquan Zheng, Serge Carrez, Ahmed Ghalgaoui and Bernard Bourguignon

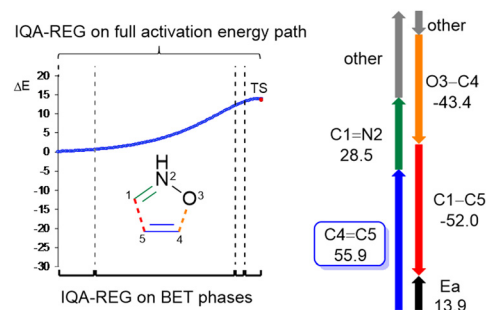


## RESEARCH PAPERS

10853

# A combined BET and IQA-REG study of the activation energy of non-polar zw-type [3+2] cycloaddition reactions

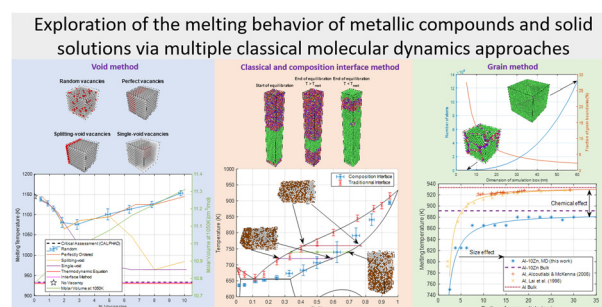
Mar Ríos-Gutiérrez,\* Fabio Falcioni, Luis R. Domingo and Paul L. A. Popelier\*



10866

# On the exploration of the melting behavior of metallic compounds and solid solutions via multiple classical molecular dynamics approaches: application to Al-based systems

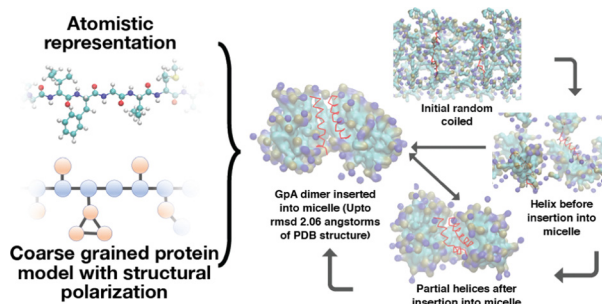
Camille Rincet, Juan-Ricardo Castillo-Sánchez, Aïmen E. Gheribi and Jean-Philippe Harvey\*



10885

# Folding and modulation of the helical conformation of Glycophorin A by point mutations

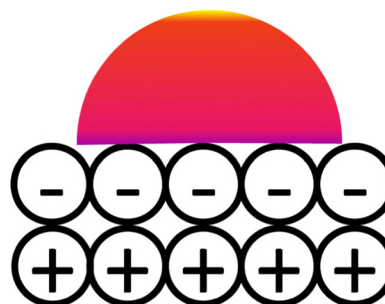
Pei-Yin Lee, Abhilash Sahoo and Silvina Matysiak\*



10894

# Accelerating water evaporation from salty droplets on polar substrate: a molecular dynamics study

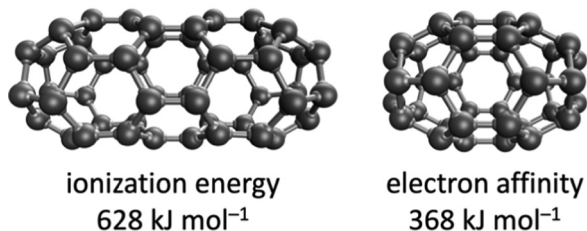
Yongfeng Huang,\* Yingzong Liang and Shun Xu\*



## RESEARCH PAPERS

10899

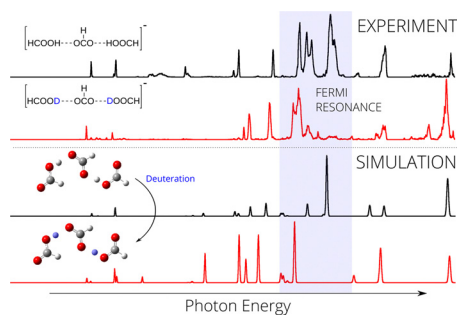
searching for small fullerenes with advantageous electronic properties



Computational insights into the singlet–triplet energy gaps, ionization energies, and electron affinities for a diverse set of 812 small fullerenes (C<sub>20</sub>–C<sub>50</sub>)

Bun Chan\* and Amir Karton

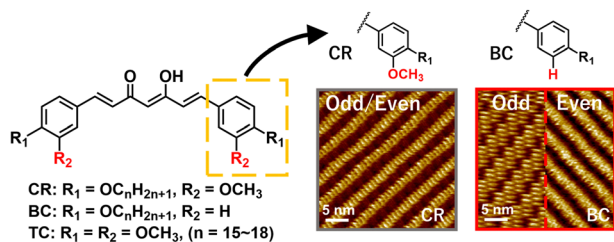
10907



Infrared action spectroscopy of the deprotonated formic acid trimer, trapped in helium nanodroplets

Martin I. Taccone, Daniel A. Thomas, Katja Ober, Sandy Gewinner, Wieland Schöllkopf, Gerard Meijer and Gert von Helden\*

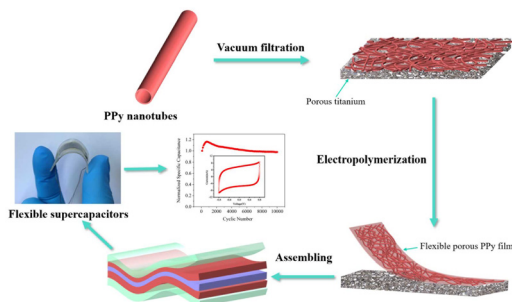
10917



Tuning the odd–even effect on two-dimensional assemblies of curcumin derivatives by alkyl chain substitution: a scanning tunnelling microscopy study

Suyi Liu, Yasuo Norikane,\* Seiji Tsuzuki, Shotaro Ito and Yoshihiro Kikkawa\*

10925



Fabrication of a flexible porous polypyrrole film with a 3D micro-nanostructure and its electrochemical properties

Jingping Wang,\* Jinan Cao, Youlong Xu,\* Haixia An and Xifei Li\*

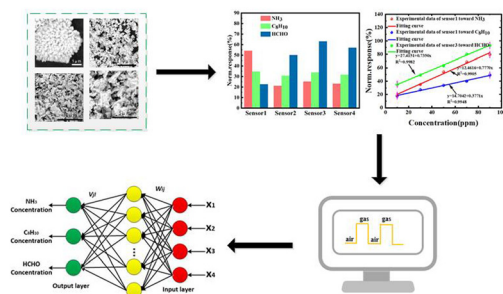


## RESEARCH PAPERS

10935

# Quantitative prediction of ternary mixed gases based on an SnO<sub>2</sub> sensor array and an SSA-BP neural network model

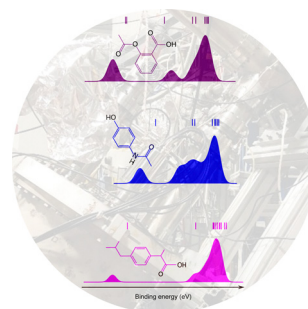
Meihua Li,\* Yunlong Gu, Yunfan Zhang, Xiaodong Gao, Shikun Ge and Guangfen Wei



10946

# A photoelectron spectroscopic investigation of aspirin, paracetamol and ibuprofen in the gas phase

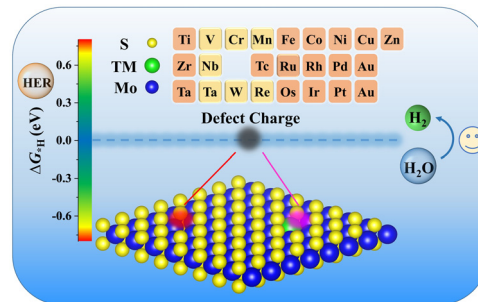
Hanan Sa'adeh,\* Kevin C. Prince, Robert Richter, Vladislav Vasilyev, Delano P. Chong and Feng Wang\*



10956

# The charge effects on the hydrogen evolution reaction activity of the defected monolayer MoS<sub>2</sub>

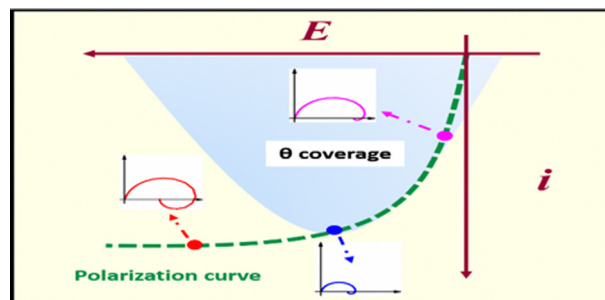
Jing Zhang, Dongying Li, Lin Ju, Gui Yang, Di Yuan, Zhenzhen Feng and Wentao Wang\*



10966

# Low-frequency inductive features in the electrochemical impedance spectra of mass-transport limited redox reactions

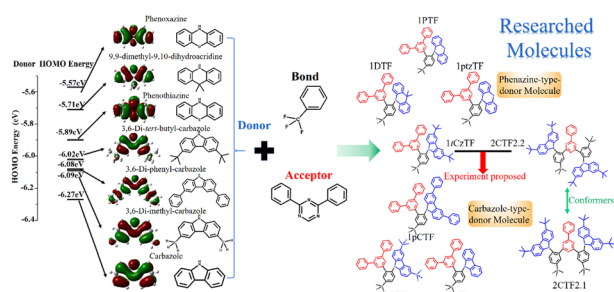
Debittree Choudhury, Rubul Das, Rajan Maurya, Geetanksha Gupta and Manoj Neergat\*





## RESEARCH PAPERS

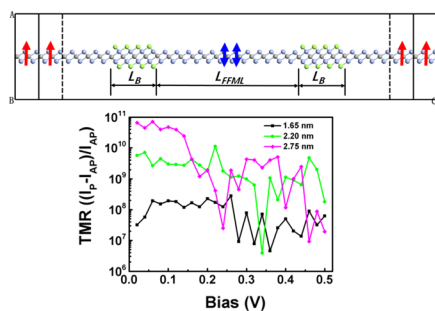
10977



**Regulating through space charge transfer in thermally activated delayed fluorescence molecules *via* donor architectures: theoretical perspective and molecular design**

Xiaorui Wang, Haipai Zou, Huanling Liu, Qingfang Mu, Kai Zhang, Yuanyuan Xu\* and Jianzhong Fan\*

10991



**Giant tunneling magnetoresistance in in-plane double-barrier magnetic tunnel junctions based on MXene Cr<sub>2</sub>C**

Hailin Yu, Mingyan Chen, Zhenguang Shao, Yongmei Tao, Xuefan Jiang, Yaojun Dong, Jie Zhang, Xifeng Yang and Yushen Liu\*

## CORRECTION

10998

**Correction: High-throughput computational screening of hypothetical metal–organic frameworks with open copper sites for CO<sub>2</sub>/H<sub>2</sub> separation**

Mengmeng Li, Weiquan Cai,\* Chao Wang and Xuanjun Wu\*

## RETRACTION

10999

**Retraction: Comparing gas transport in three polymers *via* molecular dynamics simulation**

Luke R. Anderson,\* Quan Yang and Andrew M. Ediger

