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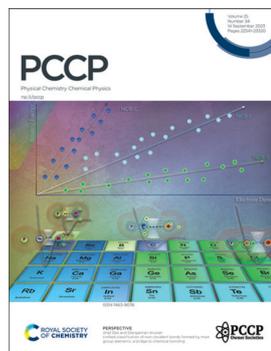
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## IN THIS ISSUE

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### Inside cover

See Samuel Ntim and Marialore Sulpizi, pp. 22619–22625. Image reproduced by permission of Samuel Ntim from *Phys. Chem. Chem. Phys.*, 2023, 25, 22619.

## EDITORIAL

22563

### Themed collection on Insightful Machine Learning for Physical Chemistry

Aurora E. Clark,\* Pavlo O. Dral,\* Isaac Tamblyn\* and Olexandr Isayev\*

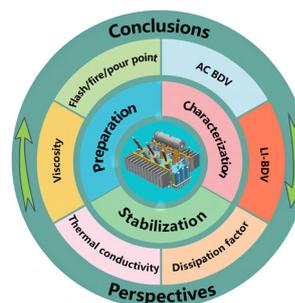


## REVIEW

22565

### Modification of insulating oils and oil-based titanium dioxide nanofluids for transformers: a review

Zilong Zhang, Fangmin Zuo, Tianzi Cai, Xingyu Gai, Li Wan, Haidan Lin, Bolin Wang\* and Haifeng Zhang\*



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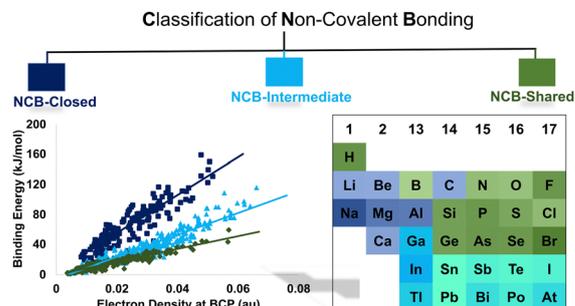


## PERSPECTIVES

22583

### Unified classification of non-covalent bonds formed by main group elements: a bridge to chemical bonding

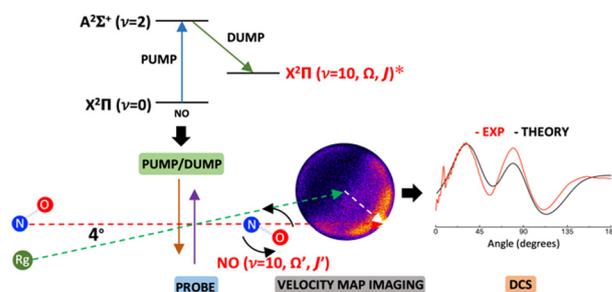
Arijit Das and Elangannan Arunan\*



22595

### Cold collisions of hot molecules

Chatura A. Perera, Chandika Amarasinghe, Hua Guo and Arthur G. Suits\*

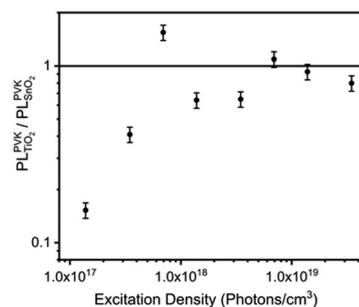


## COMMUNICATIONS

22607

### Can photoluminescence quenching be a predictor for perovskite solar cell efficiencies?

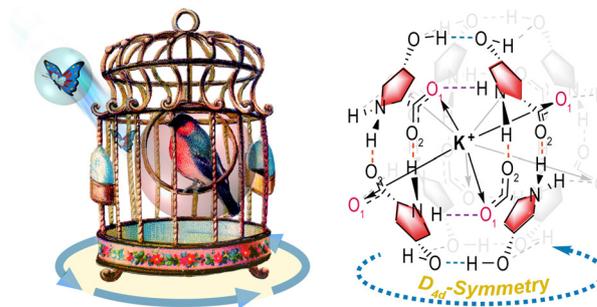
Xinjian Geng, Yawen Liu, Xianshao Zou, Erik M. J. Johansson and Jacinto Sà\*



22614

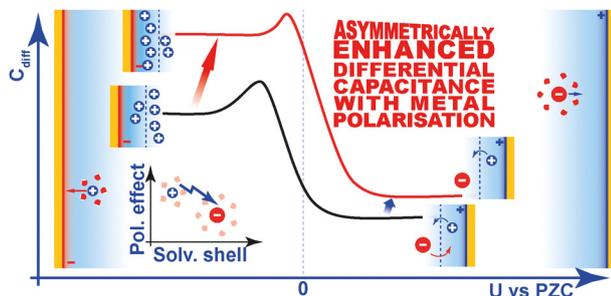
### Selective confinement of potassium, rubidium, or caesium ions in a non-covalent hydroxyproline octamer cage stabilized by *cis*-hydroxyl locks

Yameng Hou, Sijin Zhou, Xingshi Xu, Min Kou and Xianglei Kong\*



## RESEARCH PAPERS

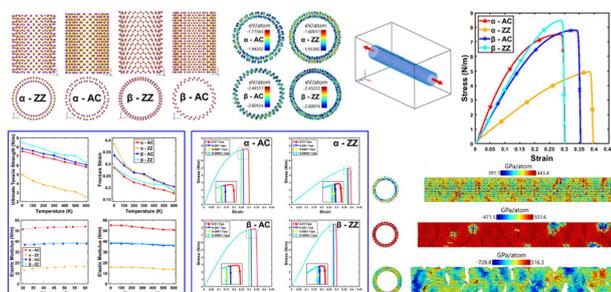
22619



### Molecular dynamics simulations of electrified interfaces including the metal polarisation

Samuel Ntim and Marialore Sulpizi\*

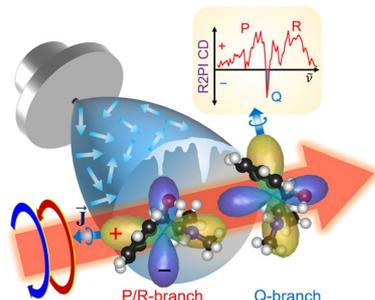
22626



### Mechanical characteristics and failure behavior of puckered and buckled allotropes of antimonene nanotubes: a molecular dynamics study

Murat Cetin and Mesut Kirca\*

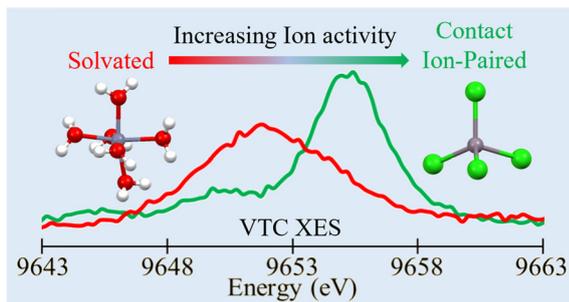
22644



### Anisotropic circular dichroism of jet-cooled chiral molecules

Changseop Jeong, Jiyeon Yun, Jiyoung Heo\* and Nam Joon Kim\*

22650



### The evolution of solvation symmetry and composition in Zn halide aqueous solutions from dilute to extreme concentrations

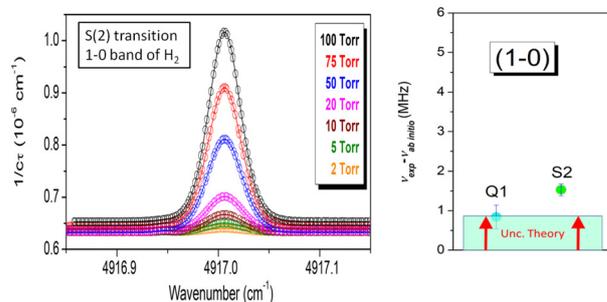
Diwash Dhakal, Darren M. Driscoll, Niranjana Govind, Andrew G. Stack, Nikhil Rampal, Gregory Schenter, Christopher J. Mundy, Timothy T. Fister, John L. Fulton, Mahalingam Balasubramanian and Gerald T. Seidler\*



22662

### Accurate absolute frequency measurement of the S(2) transition in the fundamental band of H<sub>2</sub> near 2.03 μm

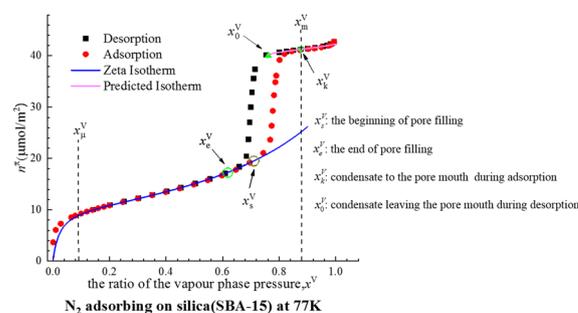
D. Mondelain,\* L. Boux de Casson, H. Fleurbaey, S. Kassi and A. Campargue



22669

### Determination of the surface properties and adsorption states of nanoporous materials using the zeta adsorption isotherm

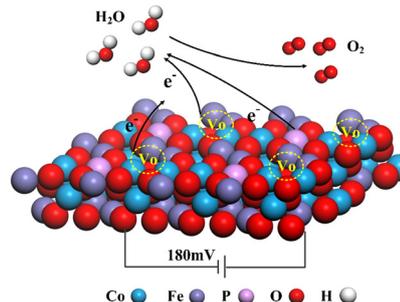
Wei Zhang, Chun-Mei Wu\* and You-Rong Li



22679

### Cold plasma synthesis of phosphorus-doped CoFe<sub>2</sub>O<sub>4</sub> with oxygen vacancies for enhanced OER activity

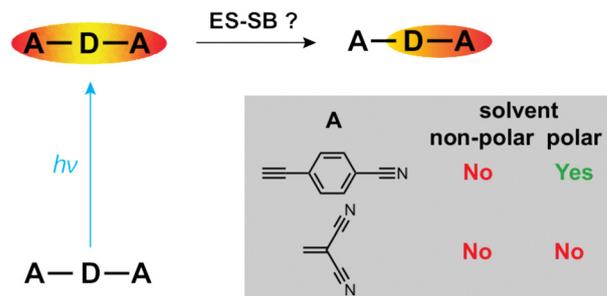
Dapeng Meng, Xiangfeng Peng, Jingxuan Zheng and Zhao Wang\*



22689

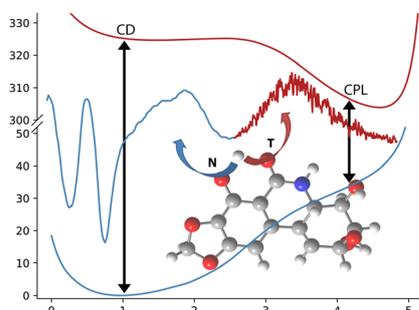
### Excited-state symmetry breaking in quadrupolar pull-push-pull molecules: dicyanovinyl vs. cyanophenyl acceptors

Pragya Verma, Mariusz Tasiar, Palas Roy, Stephen R. Meech,\* Daniel T. Gryko and Eric Vauthey\*



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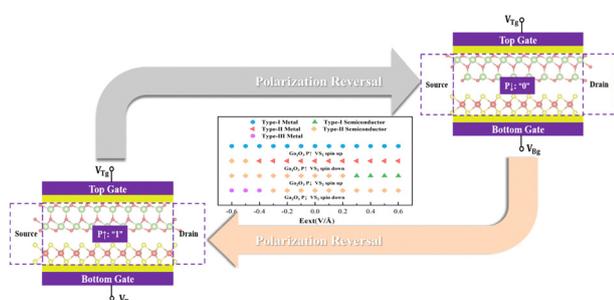
22700



### Circularly polarized luminescence of natural products lycorine and narciclasine: role of excited-state intramolecular proton-transfer and test of pH sensitivity

Giuseppe Mazzeo, Marco Fusè, Antonio Evidente, Sergio Abbate and Giovanna Longhi\*

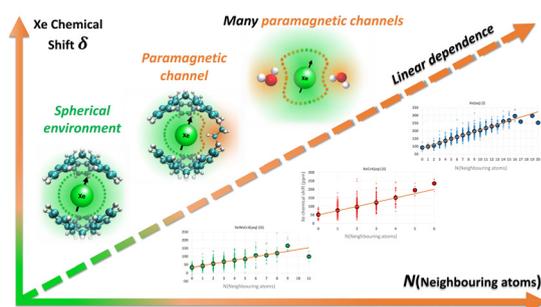
22711



### Electrostatic gating dependent multiple band alignments in ferroelectric VS<sub>2</sub>/Ga<sub>2</sub>O<sub>3</sub> van der Waals heterostructures

Yunlai Zhu, Zihan Qu, Xiaoteng Wang, Jishun Zhang, Zuheng Wu, Zuyu Xu, Fei Yang, Jun Wang and Yuehua Dai\*

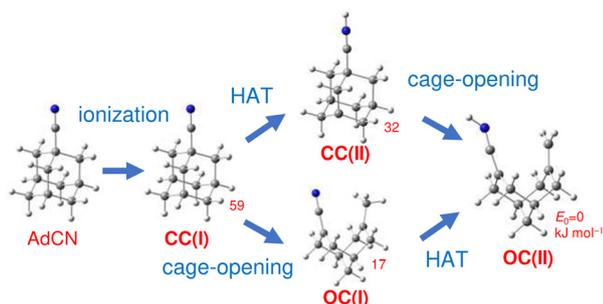
22719



### NMR chemical shift of confined <sup>129</sup>Xe: coordination number, paramagnetic channels and molecular dynamics in a cryptophane-A biosensor

Perttu Hilla\* and Juha Vaara\*

22734



### Infrared spectrum of the 1-cyanoadamantane cation: evidence of hydrogen transfer and cage-opening upon ionization

Peter Theodore Rubli and Otto Dopfer\*

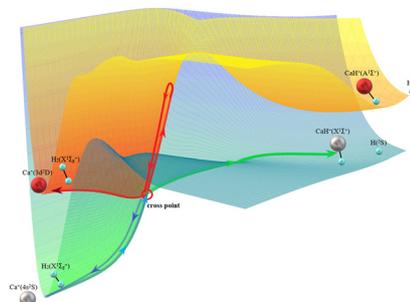


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22744

### The impact of non-adiabatic effects on reaction dynamics: a study based on the adiabatic and non-adiabatic potential energy surfaces of $\text{CaH}_2^+$

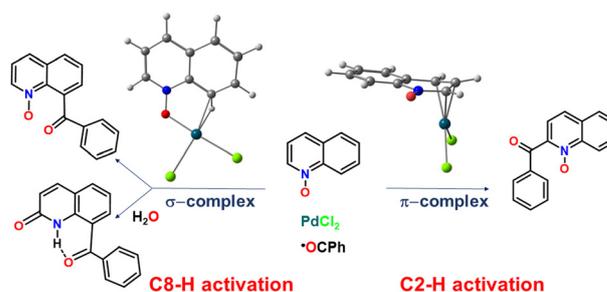
Di He,\* Wentao Li, Quanjiang Li, Shenghui Chen, Li Wang, Yanli Liu and Meishan Wang\*



22755

### C–H functionalization of quinoline N-oxides catalyzed by Pd(II) complexes: a computational study

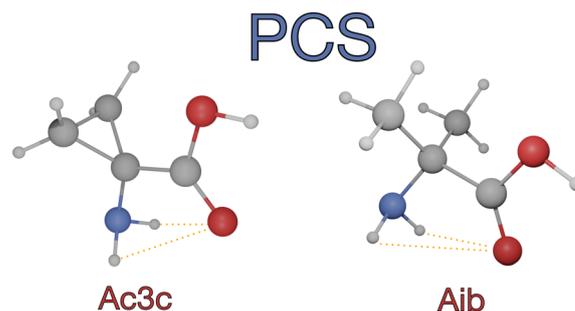
Paulo J. Costa, Frederico F. Martins, Chao Pi, Xiuling Cui and Maria José Calhorda\*



22768

### Accurate structures and spectroscopic parameters of $\alpha,\alpha$ -dialkylated $\alpha$ -amino acids in the gas-phase: a joint venture of DFT and wave-function composite methods

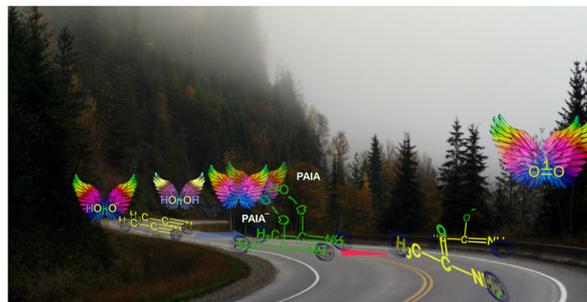
Vincenzo Barone\*



22775

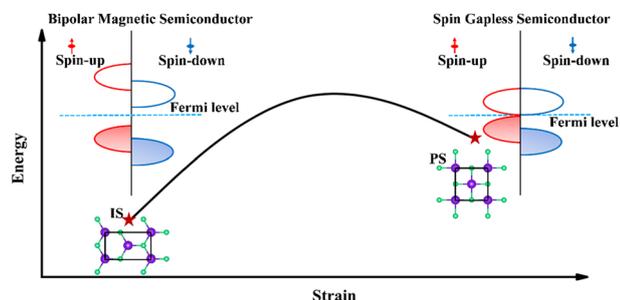
### The reaction of acetonitrile with hydrogen peroxide in alkaline medium: a DFT mechanistic study of green production of amides

Girolamo Casella,\* Silvia Carlotto, Ana P.C. Ribeiro and Luísa M.D.R.S. Martins



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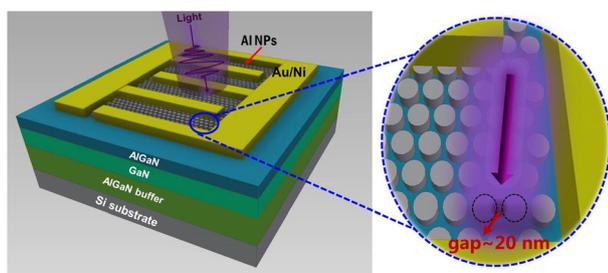
22782



### Tunable electrical properties and multiple-phases of ferromagnetic GdS<sub>2</sub>, GdSe<sub>2</sub> and Janus GdSSe monolayers

Zhihao Gao, Yuehao Yin, Yuwan Wang, Zichun Cui, Tengfei Cao, Junqin Shi and Xiaoli Fan\*

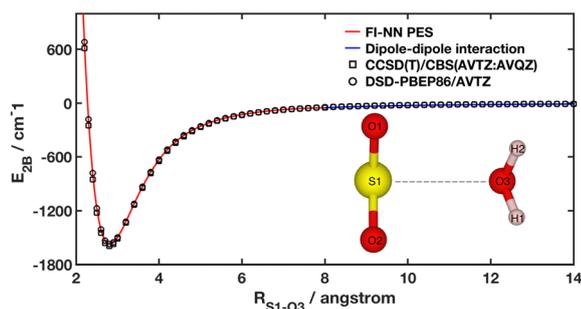
22794



### Broadband ultraviolet plasmonic enhanced AlGaIn/GaN heterojunction photodetectors with close-packed Al nanoparticle arrays

Leilei Xu, Xiaotian Ge, Zengli Huang,\* Tong Liu, Rongxin Wang, Hongwei Gao, Yu Zhou, Miao Wang, Jianfeng Wang and Ke Xu\*

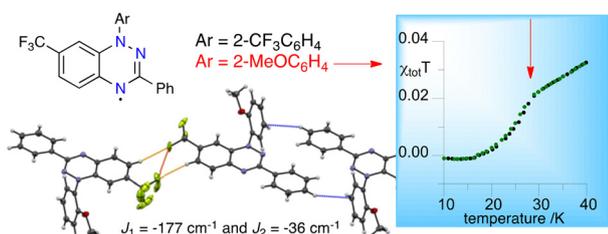
22804



### Neural network potential energy surfaces and dipole moment surfaces for SO<sub>2</sub>(H<sub>2</sub>O) and SO<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub> complexes

Liangfei Fu, Shuo Yang and Dong H. Zhang\*

22813



### Thermally induced dimensionality changes in derivatives of a "super stable" Blatter radical

Bruno Camargo, Irina Zajcewa, Anna Pietrzak, Emilia Obijalska, Jacek Szczytko and Piotr Kaszyński\*

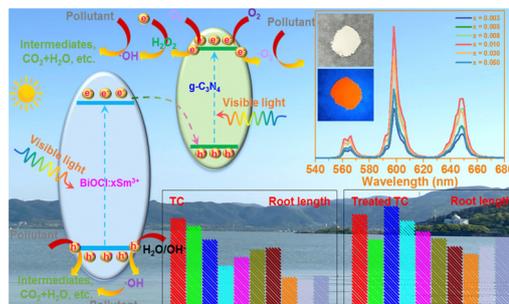


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22819

## Improved visible light triggered photocatalytic activities of BiOCl photocatalysts via a synergistic effect of doping and heterojunction engineering

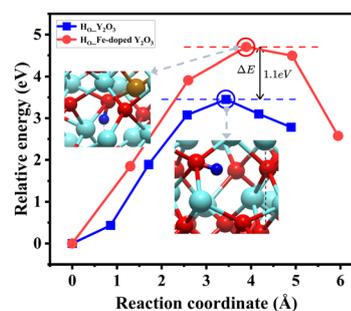
Qian Wu, Xiaoqing Lai, Xiao-Hui Ji, Hai Jiang\* and Peng Du\*



22832

Trapping and diffusion of hydrogen in iron-doped Y<sub>2</sub>O<sub>3</sub>

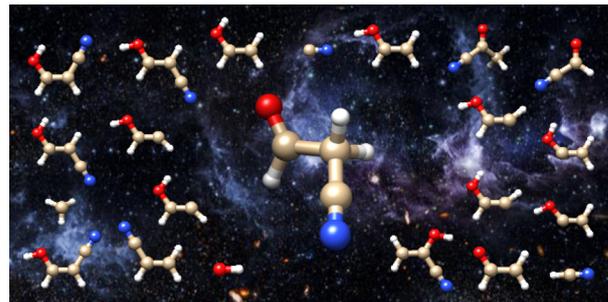
Zhenjie Liu, Zhe Feng, Chunsheng Guo,\* Yuxiang Ni, Hongyan Wang, Yuhong Xu and Changjian Tang



22840

## New prebiotic molecules in the interstellar medium from the reaction between vinyl alcohol and CN radicals: unsupervised reaction mechanism discovery, accurate electronic structure calculations and kinetic simulations

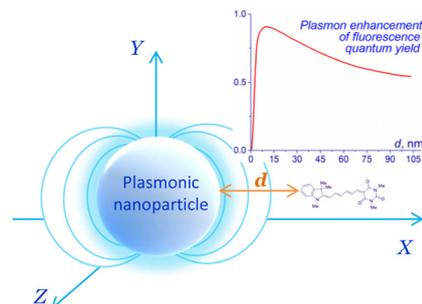
Bernardo Ballotta,\* Emilio Martínez-Núñez, Sergio Rampino and Vincenzo Barone\*



22851

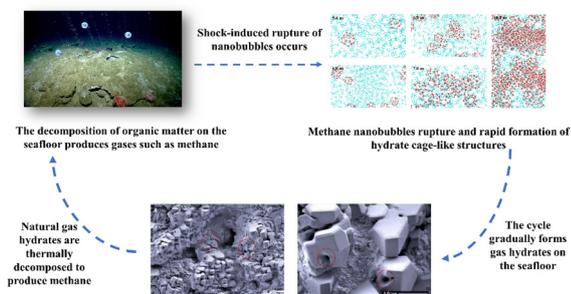
## Influence of plasmons on the luminescence properties of solvatochromic merocyanine dyes with different solvatochromism

Niyazbek Kh. Ibrayev,\* Evgeniya V. Seliverstova, Rashid R. Valiev,\* Assel E. Kanapina, Alexander A. Ishchenko, Andrii V. Kulnich, Theo Kurten and Dage Sundholm



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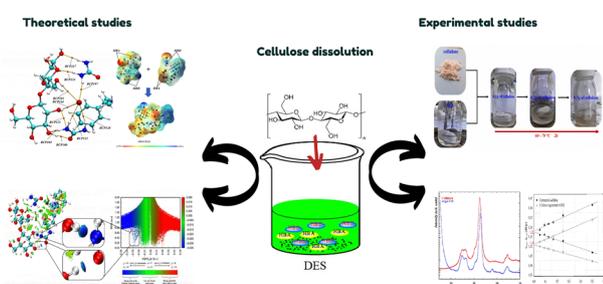
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### Molecular dynamics of the spontaneous generation mechanism of natural gas hydrates during methane nanobubble rupture

Changsheng Liu, Yan Zhang, Liang Yang,\*  
Caizhuang Wang, Xihong Lu\* and Shiwei Lin\*

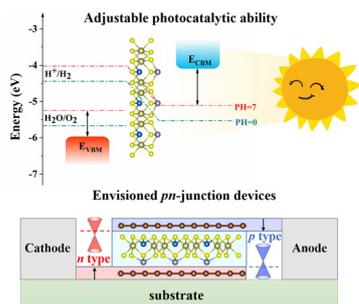
22870



### Dissolution mechanism of cellulose in a benzyltriethylammonium/urea deep eutectic solvent (DES): DFT-quantum modeling, molecular dynamics and experimental investigation

Omar Azougagh,\* Issam Jilal, Loubna Jabir,  
Hayat El-Hammi, Soumya Essayeh, Nor Mohammed,  
Nafea Achalhi, Ridouan El yousfi, Abderrahmane El Idrissi,  
Youssef El Ouardi, Katri Laatikainen, Mohamed Abou-Salama  
and Soufian El Barkary\*

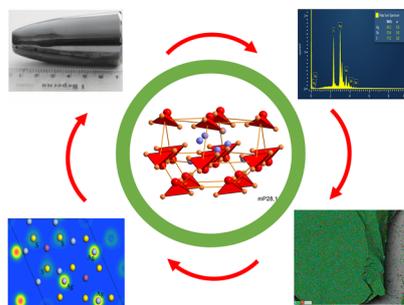
22889



### Symmetry-breaking-induced ferroelectric HfSnX<sub>3</sub> monolayers and their tunable Janus structures: promising candidates for photocatalysts and nanoelectronics

Yu Zhang, Yanqing Shen,\* Jiajia Liu, Lingling Lv,  
Min Zhou, Xin Yang, Xianghui Meng, Bing Zhang and  
Zhongxiang Zhou\*

22900



### Electronic structure and optical properties of the Ag<sub>3</sub>SbS<sub>3</sub> crystal: experimental and DFT studies

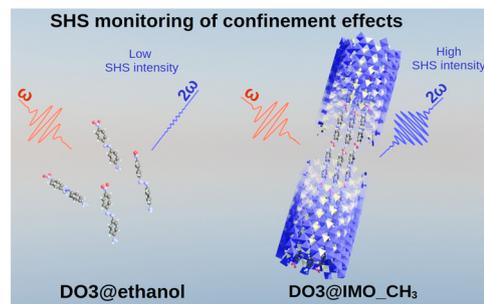
M. Ya. Rudysh,\* G. L. Myronchuk, A. O. Fedorchuk,  
O. V. Marchuk, V. M. Kordan, O. P. Kohan,  
D. B. Myronchuk and O. V. Smitiukh



22913

### Hydrophobic dye solubilization *via* hybrid imogolite nanotubes probed using second harmonic scattering

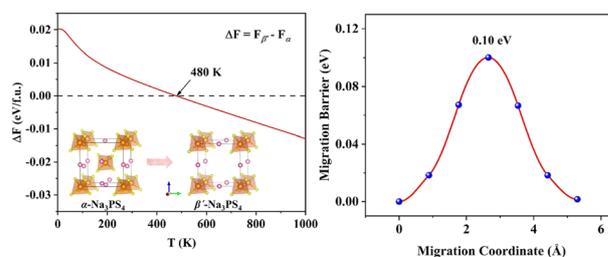
Ali Dhaini, Fadwa Alfadel Raad, Antoine Thill, Benedicte Prelot, Gaelle Martin-Gassin and Pierre-Marie Gassin\*



22920

### A novel phase of superionic conductor $\beta'$ - $\text{Na}_3\text{PS}_4$ with a large band gap and a low migration barrier

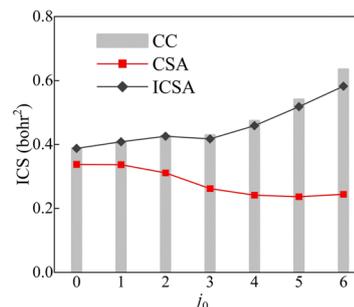
Xiaofeng Zhang, Luo Yan, Qiaoqiao Li, Yongqi Zhang\* and Liujiang Zhou\*



22927

### An effective approximation of Coriolis coupling in reactive scattering: application to the time-dependent wave packet calculations

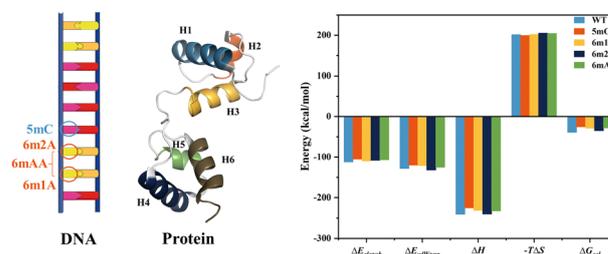
Hanghang Chen, Bayaer Buren, Zijiang Yang and Maodu Chen\*



22941

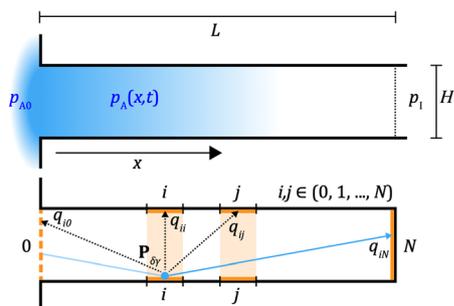
### Comprehensive analysis unveils altered binding kinetics of 5-/6-methylCytosine/adenine modifications in R2R3-DNA system

Qihang Wang, Song Luo, Danyang Xiong, Xiaole Xu, Lizhi Wang\* and Lili Duan\*



## RESEARCH PAPERS

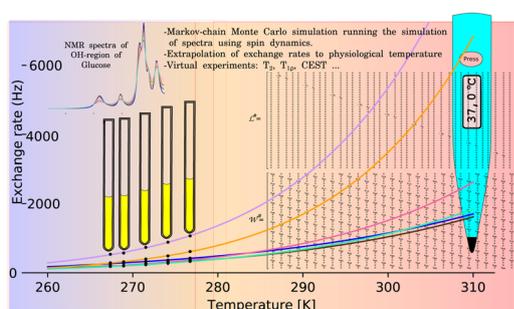
22952



### Simulation of conformality of ALD growth inside lateral channels: comparison between a diffusion–reaction model and a ballistic transport–reaction model

Jänis Järvillehto,\* Jorge A. Velasco, Jihong Yim, Christine Gonsalves and Riikka L. Puurunen\*

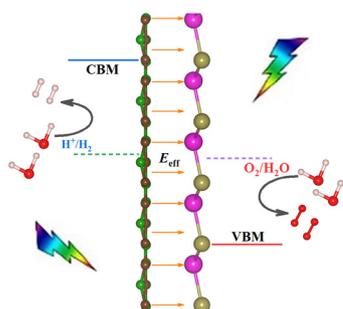
22965



### Glucose exchange parameters in a subset of physiological conditions

J. Mareš,\* J. Karjalainen, P. Håkansson, S. Michaeli and T. Liimatainen

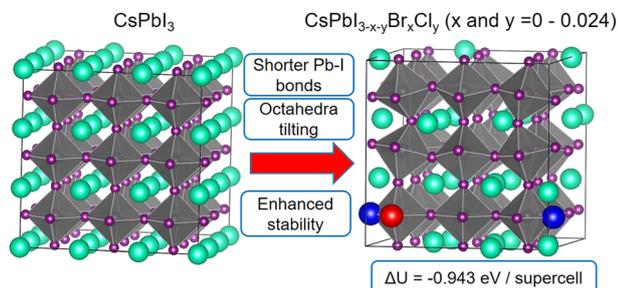
22979



### The polarized electric field of CdTe/B<sub>4</sub>C<sub>3</sub> heterostructure efficiently promotes its photocatalytic overall water splitting

Minglei Jia, Fengzhu Ren,\* Wenna Han, Pengyu Liu, Chao Jin, Xuefeng Chen, Chengxiao Peng and Bing Wang

22989



### Enhanced stability of triple-halide perovskites CsPbI<sub>3-x-y</sub>Br<sub>x</sub>Cl<sub>y</sub> (x and y = 0–0.024): understanding the role of Cl doping from *ab initio* calculations

Anu Bala\* and Vijay Kumar

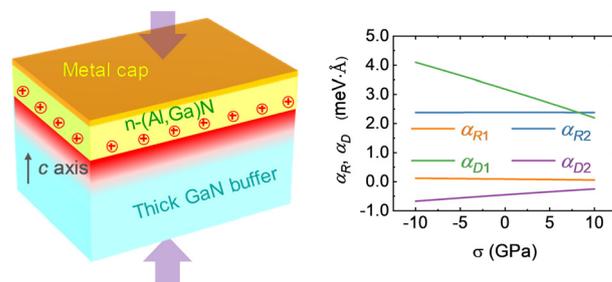


## RESEARCH PAPERS

23001

**Piezoelectric manipulation of spin–orbit coupling in a Wurtzite heterostructure**

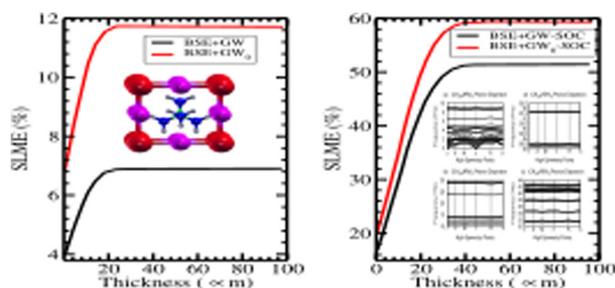
Gongwei Hu,\* Fobao Huang and Jun-Feng Liu\*



23012

**Stabilizing tetramethylammonium lead iodide perovskite and exploring its electronic and optical absorption for solar cell absorber application**

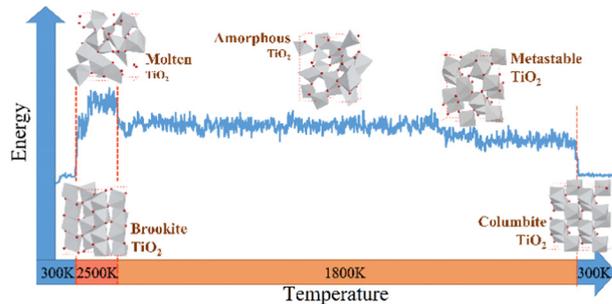
Ridwan O. Agbaoye,\* Paul O. Adebambo, Stephane Kenmoe and Gboyega A. Adebayo\*



23024

**Phase transition of titanium dioxide based on quantum dynamics**

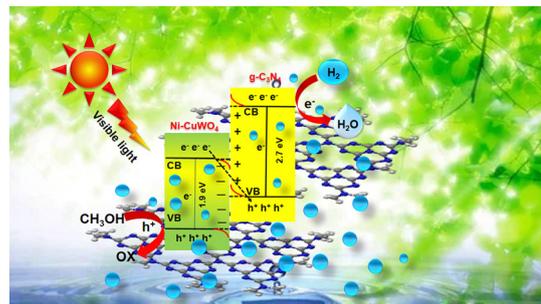
Bing Zhang, Shengbin Chen, Yang Yang, Rui Luo, Yuangu Xia, Xiaogang Wang, Qiang Lu and Bin Hu\*



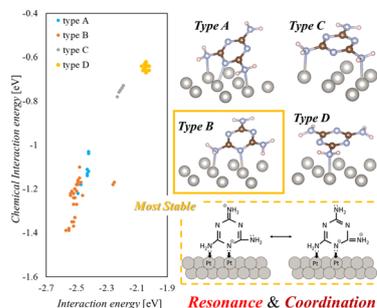
23033

**Controlled Ni doping on a g-C<sub>3</sub>N<sub>4</sub>/CuWO<sub>4</sub> photocatalyst for improved hydrogen evolution**

Purashri Basyach, Jyotirmoy Deb, Saddam Sk, Ujjwal Pal,\* Madhulekha Gogoi, G. Narahari Sastry and Lakshi Saikia\*



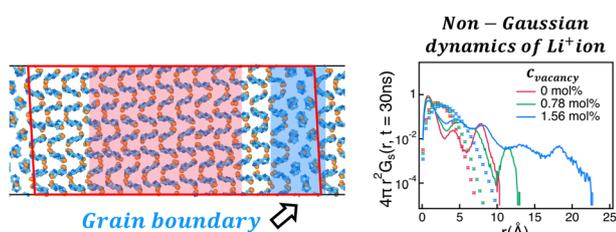
23047



### Elucidation of the mechanism of melamine adsorption on Pt(111) surface via density functional theory calculations

Kohei Tada,\* Shin-ichi Yamazaki, Masafumi Asahi and Tsutomu Ioroi

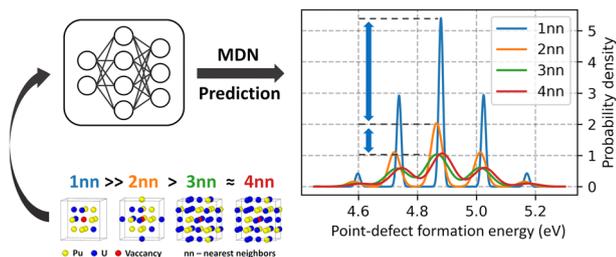
23058



### The effects of defects on the transport mechanisms of lithium ions in organic ionic plastic crystals

Hyungshick Park, Chung Bin Park and Bong June Sung\*

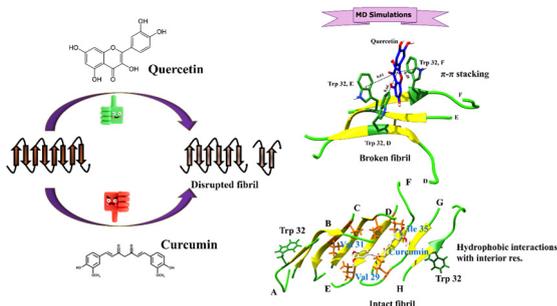
23069



### Semi-supervised generative approach to chemical disorder: application to point-defect formation in uranium-plutonium mixed oxides

Maciej J. Karcz,\* Luca Messina,\* Eiji Kawasaki, Serenah Rajaonson, Didier Bathellier, Maylise Nastar, Thomas Schuler and Emeric Bourasseau

23081



### Mechanism of the interaction of toxic SOD1 fibrils with two potent polyphenols: curcumin and quercetin

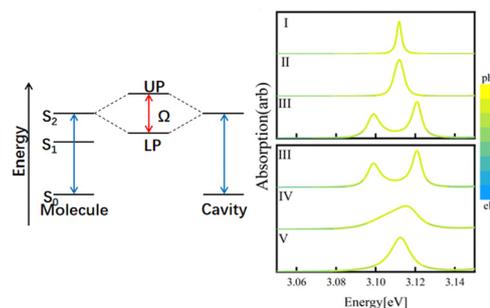
Shilpa Sharma, Vijay Raj Tomar and Shashank Deep\*



23092

## Light-responsive organic polaritons from first principles

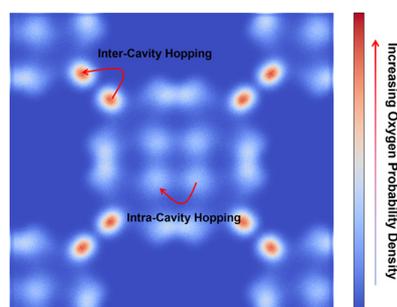
Xiongwei Guo, Xinlu Cheng\* and Hong Zhang



23100

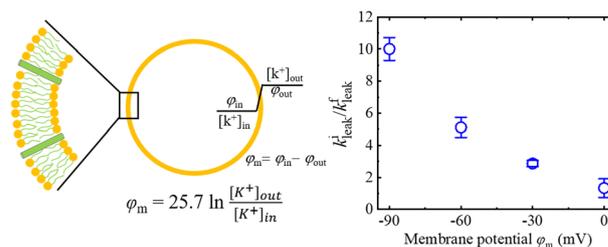
## The influence of force fields on the structure and dynamics of water confined in ZIF-8 from atomistic simulations

Jing Wang and Shi-Jie Xie\*



23111

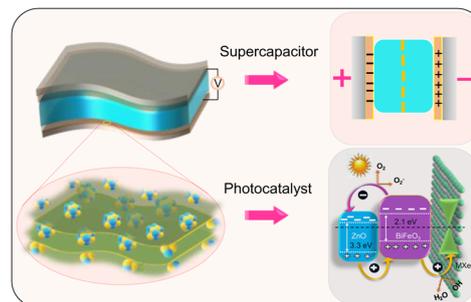
## Increase in anionic $\text{Fe}_3\text{O}_4$ nanoparticle-induced membrane poration and vesicle deformation due to membrane potential – an experimental study

Md. Moniruzzaman, Mohammad Abu Sayem Karal,\*  
Md. Abdul Wadud and Md. Mamun Or Rashid

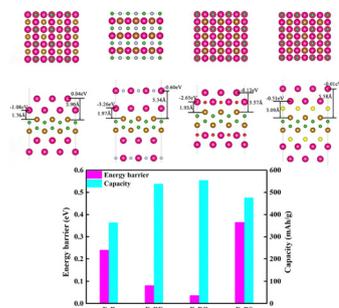
23125

## A MXene– $\text{BiFeO}_3$ – $\text{ZnO}$ nanocomposite photocatalyst served as a high-performance supercapacitor electrode

Riya Nag, Sayan Das, Debu Das, Adyam Venimadhav and Abhijit Bera\*



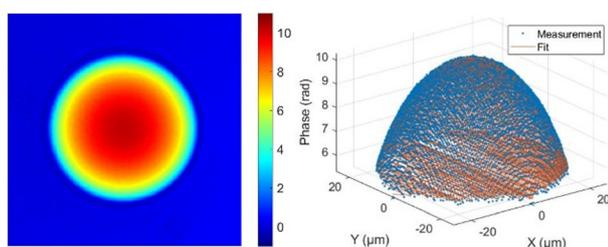
23133



## Functionalized two-dimensional iron boride compounds as novel electrode materials in Li-ion batteries

Yu Liu, Haiyan Wang,\* Yiwen Fu, Dan Li, Mengjie Wei, Qinghua Wu and Qianku Hu\*

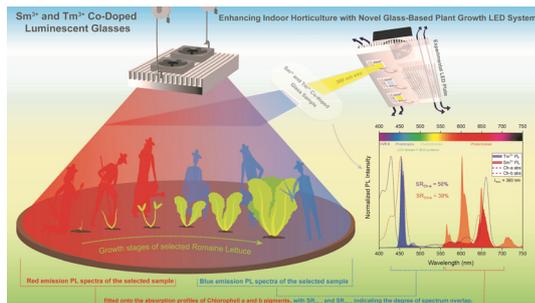
23141



## Refractive index dispersion measurement in the short-wave infrared range using synthetic phase microscopy

Melisa Nyakuchena, Cory Juntunen, Peter Shea and Yongjin Sung\*

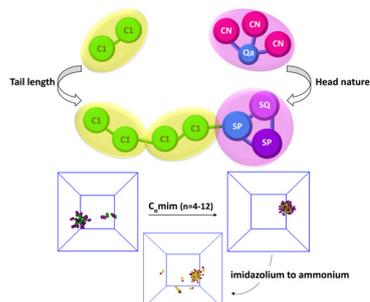
23150



## Glass-based LED system for indoor horticulture: enhanced plant growth through Sm<sup>3+</sup> and Tm<sup>3+</sup> co-doped luminescent glasses

Utku Ekim, Emre İlter, Emirhan Özcan, Yusuf Temürhan, Miray Çelikkbilek Ersundu\* and Ali Erçin Ersundu\*

23164



## The correlation between the micelle morphology of surface-active ionic liquids with self-assembly and thermodynamic characteristics: coarse-grained MD simulation and experiment

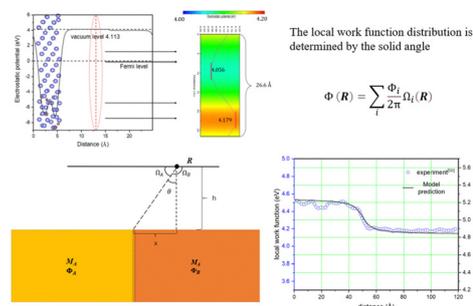
Hajar Fallah-Totkar, Ahmad Bagheri\* and Mina Maddah



23177

## Exploring the local work function of metallic materials at the nanoscale: the influence of neighboring phases

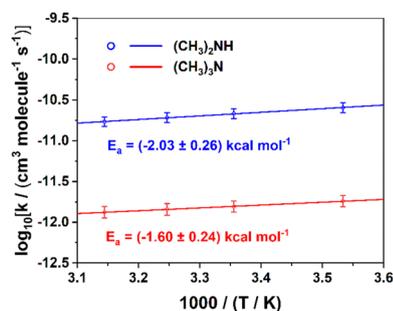
Wenjie Zhou, Chaofang Dong,\* Dihao Chen, Li Wang, Xuequn Cheng and Xiaogang Li



23187

## The simplest Criegee intermediate CH<sub>2</sub>OO reaction with dimethylamine and trimethylamine: kinetics and atmospheric implications

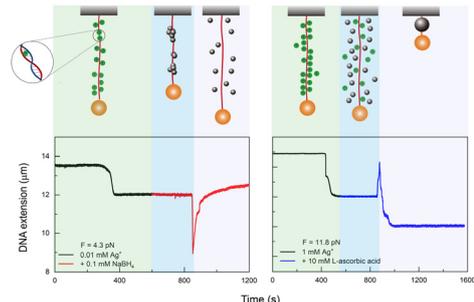
Yang Chen, Licheng Zhong, Siyue Liu, Haotian Jiang, Jiayu Shi, Yuqi Jin, Xueming Yang and Wenrui Dong\*



23197

## Reductant-dependent DNA-templated silver nanoparticle formation kinetics

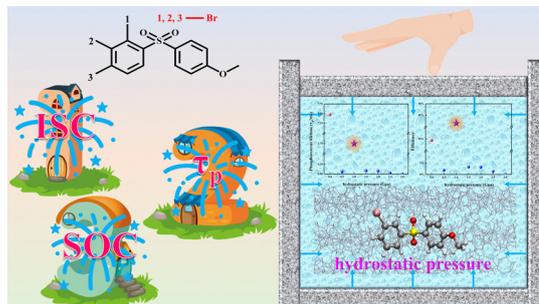
Zi-Yang Yang, Wen-Yan Jiang and Shi-Yong Ran\*



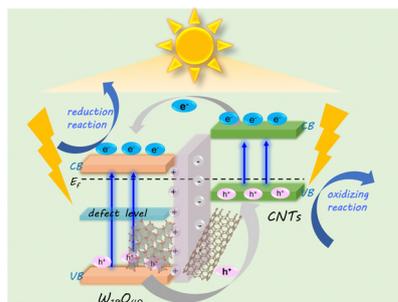
23207

## Theoretical exploration of the bromine substitution effect and hydrostatic pressure responsive mechanism for room temperature phosphorescence

Qingfang Mu, Huanling Liu, Yuzhi Song, Chuan-Kui Wang, Lili Lin, Yuanyuan Xu\* and Jianzhong Fan\*



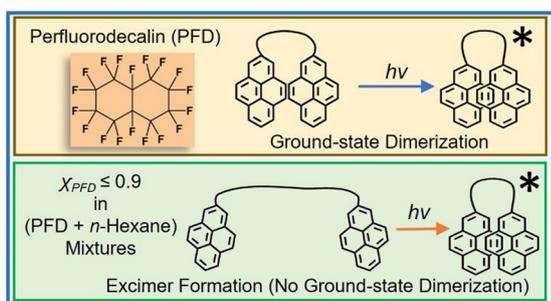
23222



### Efficient charge separation and transfer in a one-dimensional carbon nanotube/tungsten oxide p–n heterojunction composite for solar energy conversion

Yuli Ma\* and Junyu Lang\*

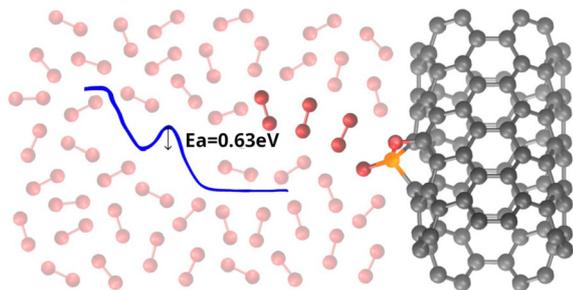
23233



### Intramolecular dimer formation reveals anomalous solvation within fluorous solvent perfluorodecalin

Deepika and Siddharth Pandey\*

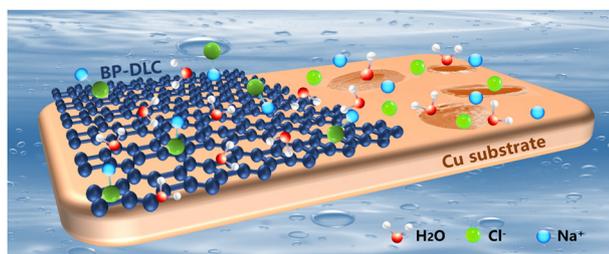
23242



### Fe-doped carbon nanotubes: towards the molecular design of new catalysts for the oxygen reduction reaction

J. L. Nuñez, G. D. Belletti, E. Colombo, R. R. Nazmutdinov and P. Quainò\*

23249



### New insights into phase transition behavior and electrochemistry corrosion of three-dimensional biphenylene

Chengyi Hou, Changhong Zhang, Sen Ming, Jiongjiong Xu, Kun Meng,\* Ju Rong, Xiaohua Yu,\* Hui Chen\* and Wei Yan

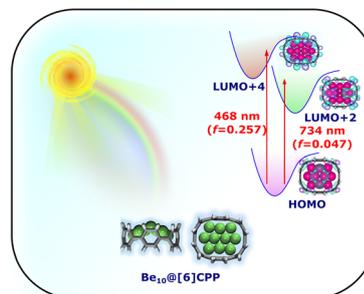


## RESEARCH PAPERS

23262

### Electronic and photophysical properties of an atomically thin bowl-shaped beryllene encapsulated inside the cavity of [6]cycloparaphenylene ( $\text{Be}_n@[\text{6}]CPP$ )

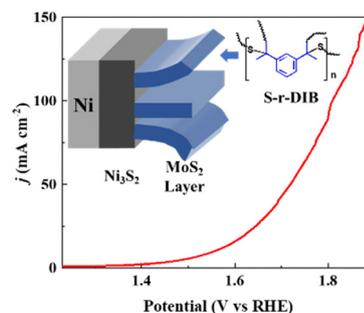
Akanksha Ashok Sangolkar, Rama Krishna Kadiyam, Mohmmad Faizan, Omshireesh Chedupaka, Raghasudha Mucherla and Ravinder Pawar\*



23277

### Polysulfide induced synthesis of a $\text{MoS}_2$ self-supporting electrode with wide-layer-spacing for efficient electrocatalytic water splitting

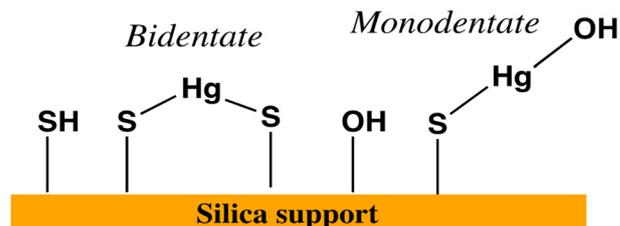
Ningbo Yu, Jianzhi Wang, Hongliang Yu, Daichunzi Yang, Wentao Luo, Xiao Lin, Yanping Liu, Ning Cai, Yanan Xue and Faquan Yu\*



23286

### Rational design of selective functionalized silica adsorbents for $\text{Hg}(\text{II})$ removal from FGD wastewater. A combined experimental and theoretical study

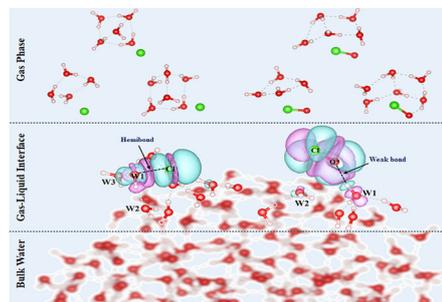
Alma Malibekova and Vadim Guliants\*



23296

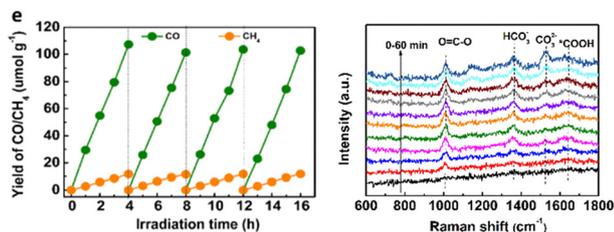
### The effects of the gas–liquid interface and gas phase on $\text{Cl}/\text{ClO}$ radical interaction with water molecules

Qi Zhang, Mohammad Hassan Hadizadeh, Yongxia Hu, Xiaoyu Zhang, Zupeng Su, Zihan Wu, Xiaotong Wang, Fei Xu,\* Yanhui Sun, Qingzhu Zhang and Wenxing Wang



## RESEARCH PAPERS

23306



### Cu-doped mesoporous SnO<sub>2</sub> nanoparticles with rich grain boundaries and oxygen vacancies for photocatalytic CO<sub>2</sub>-to-CO conversion

Guohui Li, Pengyu Li, Zhi Ge, Dawei Yan, Wei Sun, Yuanyuan Sun\* and Xiaoxia Zhou

## CORRECTIONS

23314

### Correction: The reaction of acetonitrile with hydrogen peroxide in alkaline medium: a DFT mechanistic study of green production of amides

Girolamo Casella,\* Silvia Carlotto, Ana P. C. Ribeiro and Luísa M. D. R. S. Martins

23316

### Correction: Time-resolved infra-red studies of photo-excited porphyrins in the presence of nucleic acids and in HeLa tumour cells: insights into binding site and electron transfer dynamics

Páraic M. Keane,\* Clara Zehe, Fergus E. Poynton, Sandra A. Bright, Sandra Estayalo-Adrián, Stephen J. Devereux, Paul M. Donaldson, Igor V. Sazanovich, Michael Towrie, Stanley W. Botchway, Christine J. Cardin, D. Clive Williams, Thorfinnur Gunnlaugsson, Conor Long,\* John M. Kelly\* and Susan J. Quinn\*

