

## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(18) 9287–9896 (2025)



**Cover**  
See Dana Bloß *et al.*, pp. 9329–9335. Image reproduced by permission of Dana Bloß from *Phys. Chem. Chem. Phys.*, 2025, 27, 9329. Background generated with AI.



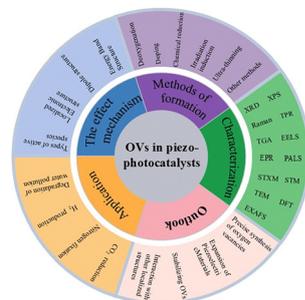
**Inside cover**  
See Chun-Liang Lin, Jyh-Pin Chou, Meng-Fan Luo *et al.*, pp. 9336–9349. Image reproduced by permission of Wan-Hsin Chen and Yu-Yao Hsia from *Phys. Chem. Chem. Phys.*, 2025, 27, 9336.

## REVIEW

9304

### Oxygen vacancies in piezo-photocatalysts: synthesis, characterization, effect mechanism and application

Huaibao Qiu, Fan Wu, Jie Yuan, Wenhui Feng\* and Xiaoqing Qiu\*

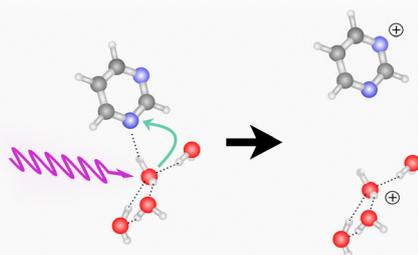


## RESEARCH PAPERS

9329

### Interplay of protection and damage through intermolecular processes in the decay of electronic core holes in microsolvated organic molecules

Dana Bloß,\* Nikolai V. Kryzhevoi, Jonas Maurmann, Philipp Schmidt, André Knie, Johannes H. Viehmann, Catmarina Küstner-Wetekam, Sascha Deinert, Gregor Hartmann, Florian Trinter, Lorenz S. Cederbaum, Arno Ehresmann, Alexander I. Kuleff and Andreas Hans



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Fundamental questions  
Elemental answers

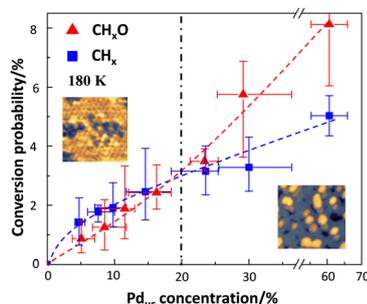


## RESEARCH PAPERS

9336

Decomposition of methanol activated by surface under-coordinated Pd on layered PdTe<sub>2</sub>

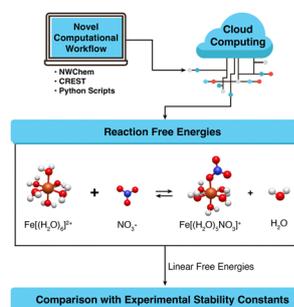
Jing-Wen Hsueh, Lai-Hsiang Kuo, Po-Han Chen, Wan-Hsin Chen, Chi-Yao Chuang, Chia-Nung Kuo, Chin-Shan Lue, Hung-Wei Shiu, Bo-Hong Liu, Chia-Hsin Wang, Yao-Jane Hsu, Chun-Liang Lin,\* Jyh-Pin Chou\* and Meng-Fan Luo\*



9350

## On the stability constants of metal–nitrate complexes in aqueous solutions

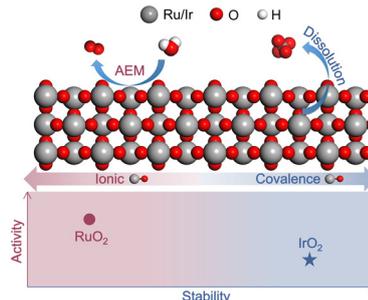
Mohammadhasan Dinpajooh,\* Greta L. Hightower, Richard E. Overstreet, Lori A. Metz, Neil J. Henson, Niranjana Govind, Andrew M. Ritzmann and Nicolas E. Uhnak\*



9369

Metal–oxygen bonding characteristics dictate activity and stability differences of RuO<sub>2</sub> and IrO<sub>2</sub> in the acidic oxygen evolution reaction

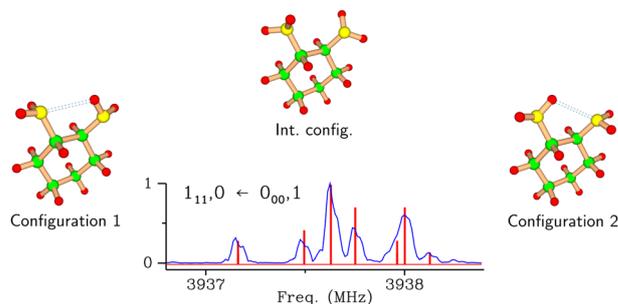
Longdan Tang, Xia Chen, Zhuoyang Xie, Qiong Xiang, Jin Liu, Li Li\* and Zidong Wei



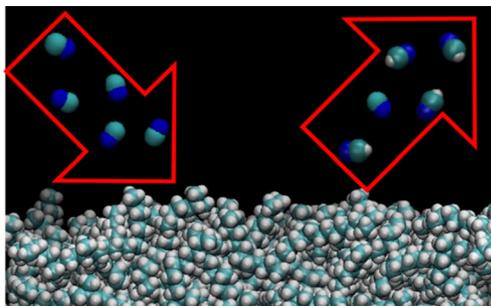
9379

Hyperfine structure-tunneling coupling in *trans*-1,2-cyclohexanediamine revealed by rotational spectroscopy

L. H. Coudert,\* Fan Xie and Melanie Schnell



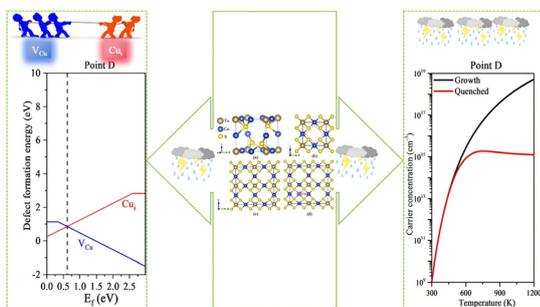
9387



### Reactive uptake *via* inelastic scattering of CN radicals at a liquid hydrocarbon surface

Paul D. Lane, Katya E. Moncrieff, Stuart J. Greaves, Kenneth G. McKendrick and Matthew L. Costen\*

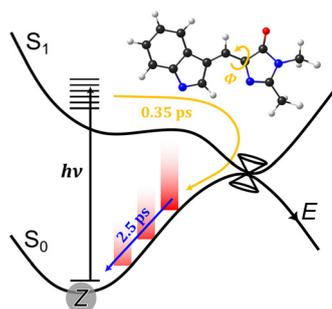
9396



### Strong compensation effects related to the empty channel in p-type transparent conductive material $\text{Cu}_3\text{TaS}_4$ : a first-principles study

Yang Xue, Zhihao Zhuo, Changqing Lin and Dan Huang\*

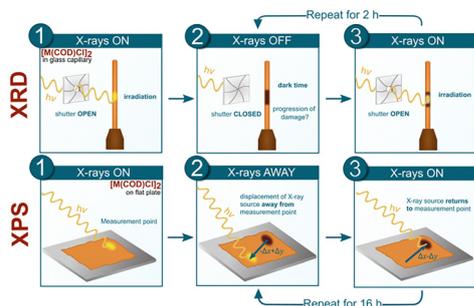
9407



### Ultrafast photophysics of the cyan fluorescent protein chromophore in solution

Anam Fatima, Eleanor K. Ashworth, Isabelle Chambrier, Andrew N. Cammidge, Giovanni Bressan, Stephen R. Meech and James N. Bull\*

9417



### Investigating discontinuous X-ray irradiation as a damage mitigation strategy for $[\text{M}(\text{COD})\text{Cl}]_2$ catalysts

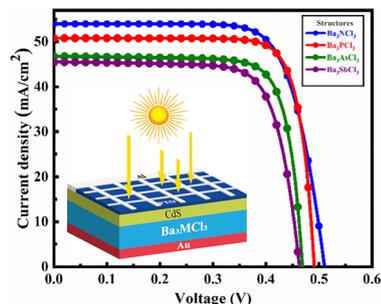
Nathalie K. Fernando, Claire A. Murray, Amber L. Thompson, Katherine Milton, Andrew B. Cairns and Anna Regoutz\*



9429

### Exploring the influence of M-anion modifications on the physical properties of lead-free novel halide inorganic compounds $Ba_3MCl_3$ ( $M = N, P, As, Sb$ )

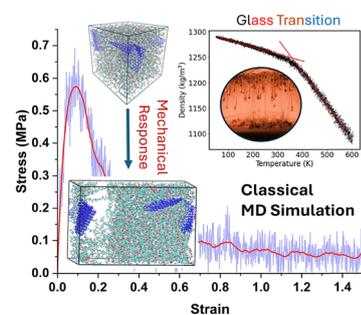
Md. Al Ijjul Islam, Md. Ferdous Rahman,\* Tanvir Al Galib, Mustafa K. A. Mohammed,\* Sagar Bhattarai and Ahmad Irfan



9448

### Revealing thermophysical and mechanical responses of graphene-reinforced polyvinyl alcohol nanocomposites using molecular dynamics simulations

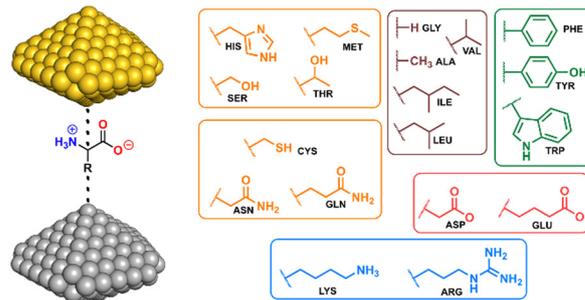
Pabitra Narayan Samanta, Devashis Majumdar and Jerzy Leszczynski\*



9463

### Noncovalent binding phenomena in the adsorption of amino acids on Ag/Au surfaces: a theoretical approach

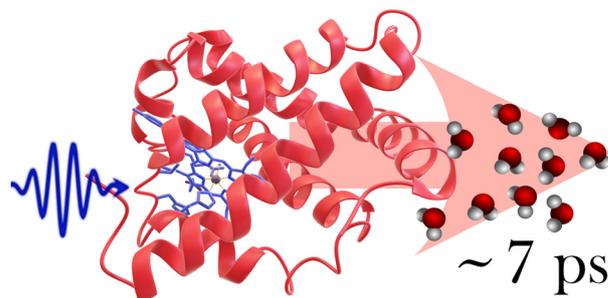
Catalina Nicolau, Sergi Burguera, María de las Nieves Piña and Antonio Bauzá\*



9470

### Internal vibrational energy redistribution precedes energy dissipation into the solvent upon photoexcitation of heme proteins

Adrian Buchmann, Luigi Caminiti, Lion Luca Stiewe, Sebastian Jung, David M. Leitner and Martina Havenith\*



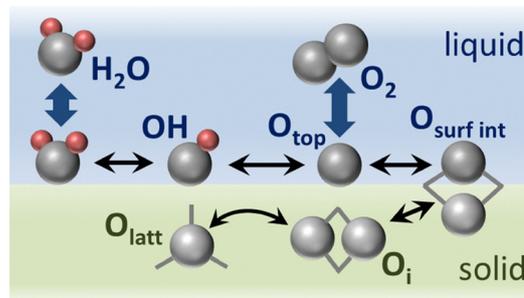


## RESEARCH PAPERS

9522

**Reactions of fluid and lattice oxygen mediated by interstitial atoms at the  $\text{TiO}_2(110)$ –water interface**

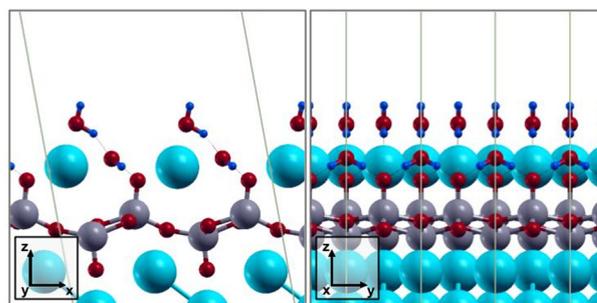
Heonjae Jeong, Ian I. Suni, Raylin Chen, Marina Miletic, Xiao Su and Edmund G. Seebauer\*



9537

**Clean and hydrated low-index  $\text{Rb}_2\text{Ti}_2\text{O}_5$  surfaces**

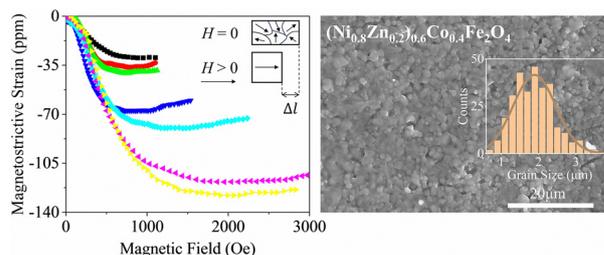
Guillaume Benas,\* Sofia De Sousa Coutinho, Brigitte Leridon and Fabio Finocchi



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**Highly sensitive magnetostrictive  $\text{NiZnCo}$  ferrites for low magnetic field sensor applications**

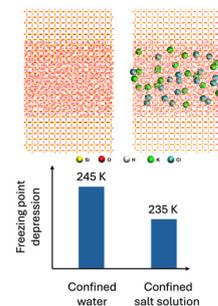
Yiyang Cui, Xiaokang Yang, Haofang Ma, Caiyun Qi, Baorui Xia\* and Daqiang Gao



9562

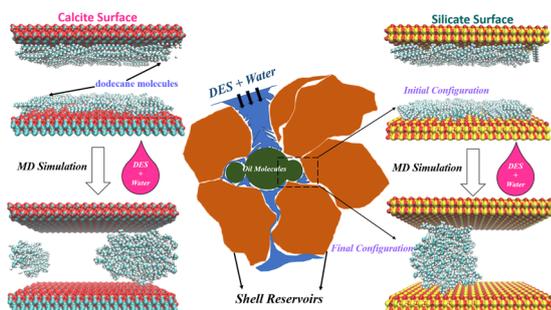
**Elucidating molecular scale interactions underlying the freezing behavior of salt solutions in silica nanopores**

Sohaib Mohammed, Hassnain Asgar, Yang Jia, Rituparna Hazra, Prince Ochonma, Chris J. Benmore and Greeshma Gadikota\*



## RESEARCH PAPERS

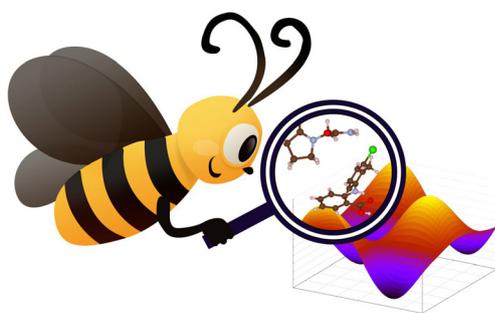
9573



### Enhanced oil recovery promoted by aqueous deep eutectic solvents on silica and calcite surfaces: a molecular dynamics study

Alok Kumar, Swasti Medha, Devargya Chakraborty, Debashis Kundu and Sandip Khan\*

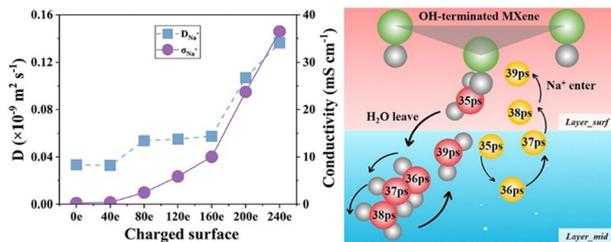
9590



### Artificial bees collect diverse conformers of small organic molecules

Anastasiia A. Smirnova,\* Maxim D. Yablonskiy, Ekaterina I. Marchenko, Nikolai G. Andreadi and Artem A. Mitrofanov

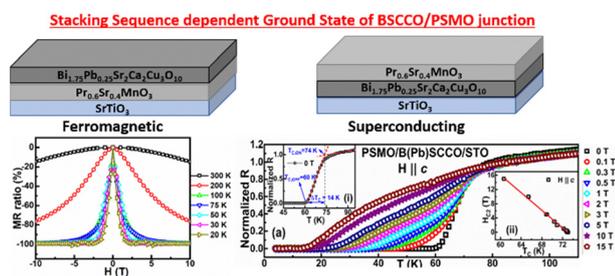
9599



### Surface charge-driven sodium-ion migration and secondary desolvation in MXene nanoconfinement

Lei Li, Huihong Wang and Zhu Liu\*

9607



### Studies on the proximity effect in Bi-based high temperature superconductor/manganite heterostructures

Gayathri V.,\* E. P. Amaladass, A. T. Sathyanarayana, T. Geetha Kumary, R. Pandian, Pooja Gupta, Sanjay K. Rai and Awadhesh Mani\*

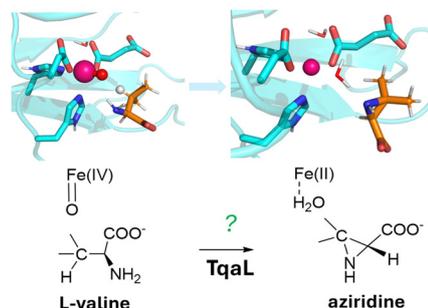


## RESEARCH PAPERS

9620

### Unusual mechanism of aziridine biosynthesis catalysed by the $\alpha$ KG-dependent non-heme enzyme TqaL

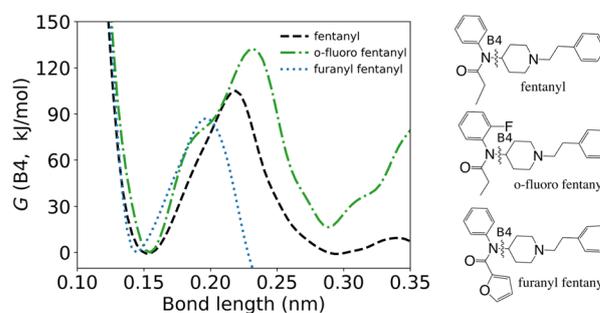
Warispreet Singh\* and Meilan Huang\*



9631

### Thermal degradation energetics of fentanyl and its analogues: furanyl fentanyl and *ortho*-fluoro fentanyl

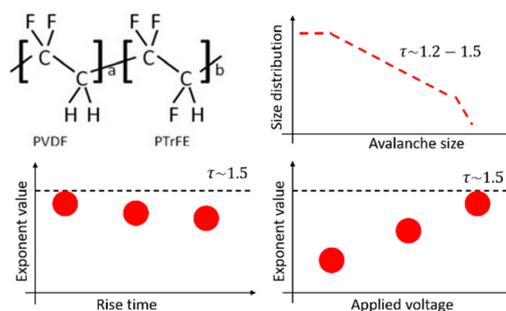
Bharat Poudel, Joshua J. Whiting, Juan M. Vanegas\* and Susan B. Rempe\*



9637

### Barkhausen noise in the organic ferroelectric copolymer P(VDF:TrFE)

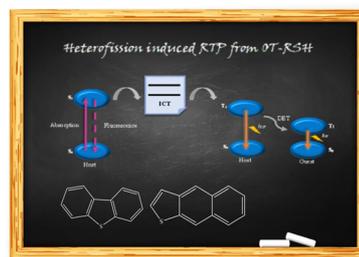
Andrey Alekseevich Butkevich, Marcel Hecker, Toni Seiler and Martijn Kemerink\*



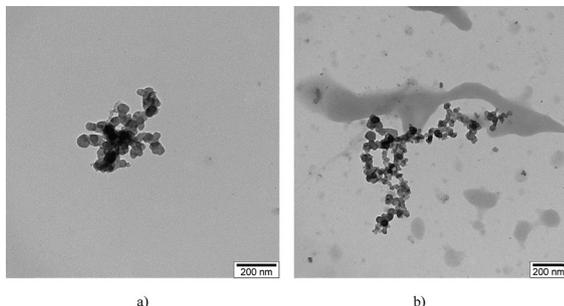
9645

### Heterofission-induced room temperature phosphorescence from range-separated hybrids: in search of the qualified blending components

Fatemeh Vaziri Alamdarloo and Mojtaba Alipour\*



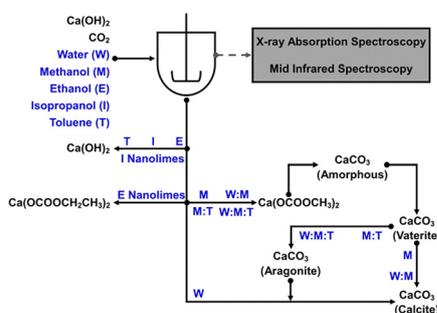
9659



### Effect of nanoparticle concentration on the crystallinity, vibrational dynamics and morphology of PS/TiO<sub>2</sub> nanocomposites: a comprehensive study

A. Rahimli\* and M. Jafarov

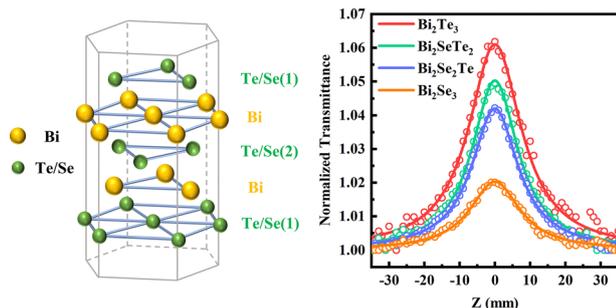
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### How non-aqueous media direct the reaction of Ca(OH)<sub>2</sub> with CO<sub>2</sub> to different forms of CaCO<sub>3</sub>: *operando* mid-infrared and X-ray absorption spectroscopy studies

Thokozile A. Kathyola, Sin-Yuen Chang, Elizabeth A. Willneff, Colin J. Willis, Giannantonio Cibin, Paul Wilson, Anna B. Kroner, Elizabeth J. Shotton, Peter J. Dowding and Sven L. M. Schroeder\*

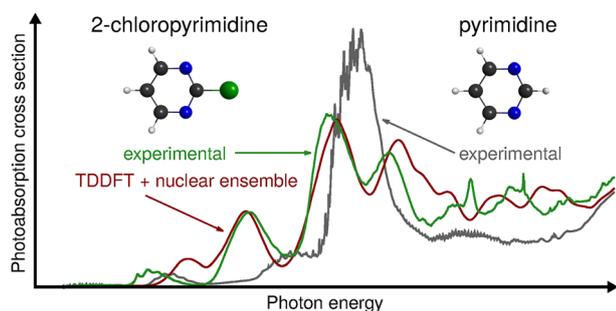
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### Tunable structural and optical properties of Bi<sub>2</sub>Se<sub>x</sub>Te<sub>3-x</sub> thin films: implications for nonlinear optical applications

Tengfei Zhang, Shenjin Wei, Shubo Zhang, Menghan Li, Jiawei Wang, Jingze Liu, Junhua Wang, Ertao Hu and Jing Li\*

9687



### Vacuum ultraviolet spectroscopy of pyrimidine derivatives: the effect of halogenation

Fábris Kossoski,\* Mónica Mendes,\* Ana I. Lozano, Rodrigo Rodrigues, Nykola C. Jones, Søren V. Hoffmann and Filipe Ferreira da Silva

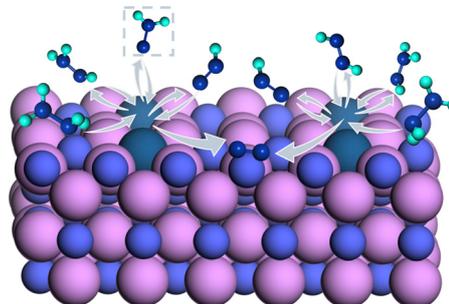


## RESEARCH PAPERS

9702

### Transition metal-doped cobalt phosphide for efficient hydrazine oxidation: a density functional theory study

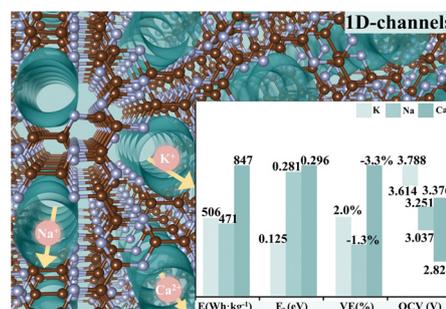
Zixin Zhou, Min Zhou, Xiaobin Liao, Mengjun Zhou,\*  
Xiaolin Liu,\* Qian Liu\* and Yan Zhao\*



9711

### Layered carbon nitride bulk as a versatile cathode material for fast ion batteries

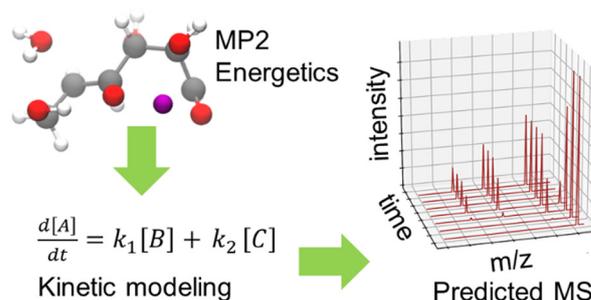
Jiaqi Zhang, Jiaxin Jiang, Hongyan Guo,\* Xiaowei Sheng,  
Weiyi Wang, Zhiwen Zhuo\* and Ning Lu\*



9721

### Collision-induced dissociation mass spectra of Na<sup>+</sup>-tagged aldohexoses simulated from first-principles calculations

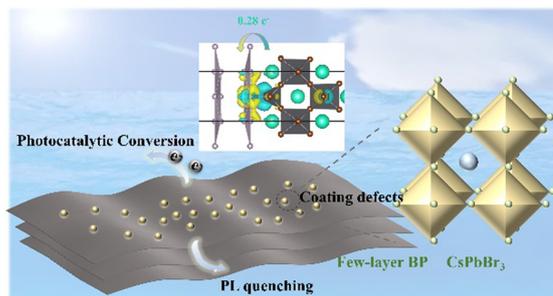
Hai Thi Huynh, Jer-Lai Kuo and Cheng-chau Chiu\*



9732

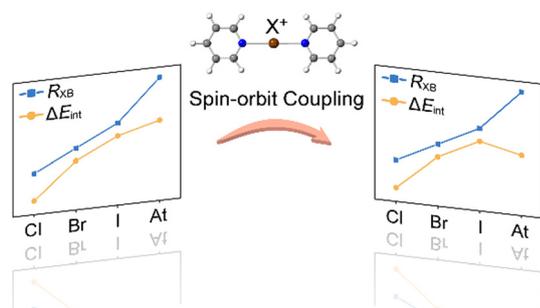
### The carrier dynamics for self-assembled black phosphorus and perovskite nanocrystals enable photocatalytic conversion

Jing Ji, Hang Yin,\* Xin Zhou, Bingxi Song, Xuhui Feng,  
Peiqing Cai, Laishun Qin,\* Yuexiang Huang,  
Jianyong Liu and Da Chen\*



## RESEARCH PAPERS

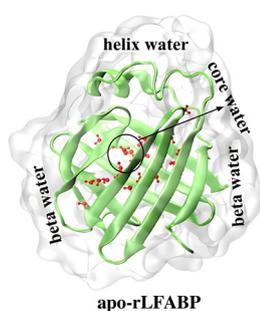
9741



### The halogen(II) complex of astatine: a theoretical perspective on structural and bonding properties

Hao Luo, Ze-Kai Li, Zhuo-Wei Zhang, Lin-Jia Chen and Jing Su\*

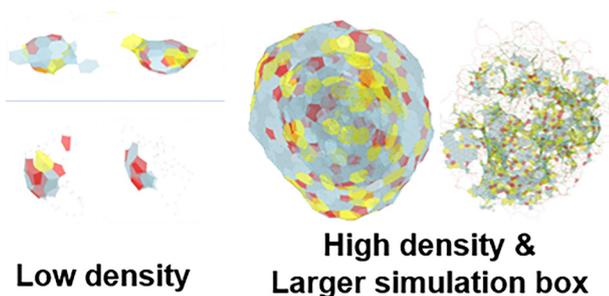
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### Elucidating the microscopic properties of a $\beta$ -barrel protein and the solvent confined in and around it

Gourab Saha and Sanjoy Bandyopadhyay\*

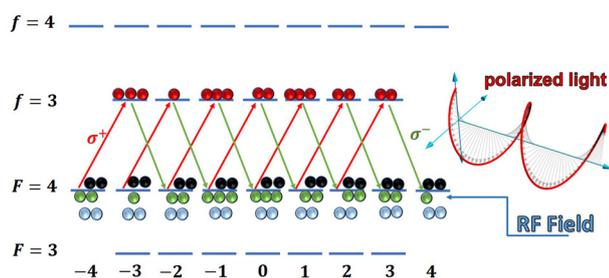
9767



### Unveiling fullerene formation and interconversion through molecular dynamics simulations with deep neural network potentials

Yanbo Han, Mengyang Li,\* Masahiro Ehara and Xiang Zhao\*

9774



### Investigation of optical pumping in cesium atoms with circularly polarized light and radio-frequency field: a theoretical approach

Hossein Davoodi Yeganeh and Zahra Shaterzadeh-Yazdi\*

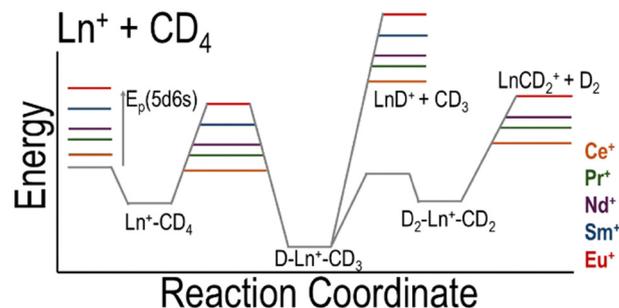


## RESEARCH PAPERS

9781

### An inductively coupled plasma tandem mass spectrometry investigation of the activation of methane by lanthanide cations

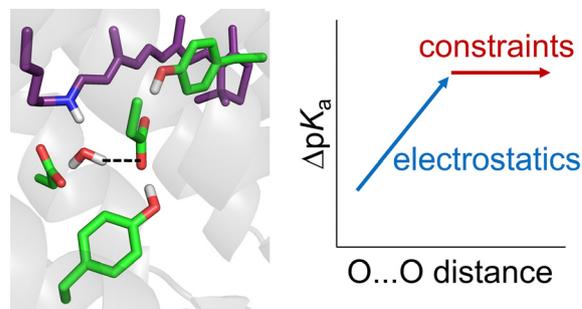
Amanda R. Bubas, Amanda D. French, Kali M. Melby, Michael J. Rodriguez and Richard M Cox\*



9794

### Determinants of hydrogen bond distances in proteins

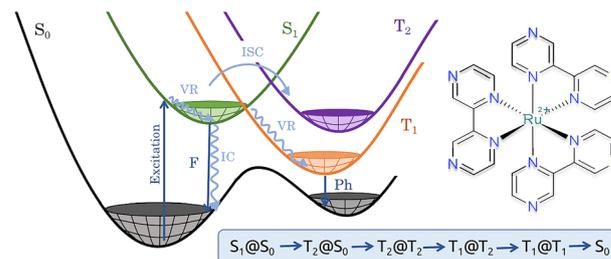
Masaki Tsujimura,\* Hiroshi Ishikita and Keisuke Saito\*



9806

### Understanding the excited state decay mechanism of complex systems: a general first-order kinetic model

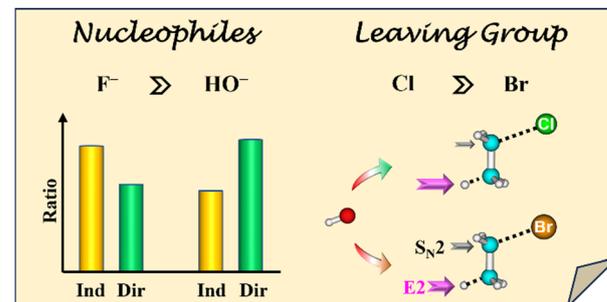
Aline de Souza Bozzi, Rita de Cássia Oliveira Sebastião and Willian Ricardo Rocha\*



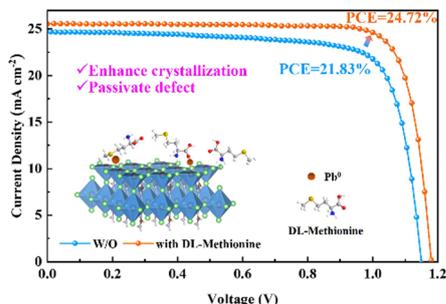
9817

### Competitive dynamics of elimination and substitution reactions modulated using nucleophiles and leaving groups

Gang Fu, Hongyi Wang, Wenqing Zhen, Xin Zhou, Li Yang\* and Jiaxu Zhang\*



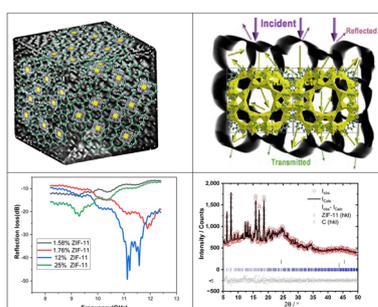
9828



### High-efficiency and stable perovskite solar cells via DL-methionine-enhanced crystallization and defect passivation

Xiaolan Li, Yanwei Xu, Fuxing Chen, Dongxing Lu, Yajun Zhu and Cong Li\*

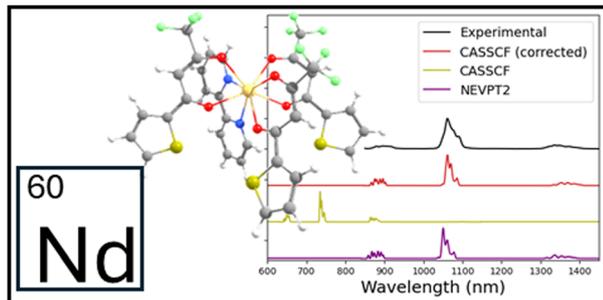
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### Highly compatible ZIF-11 MOF-embedded carbon foam nanocomposites for efficient electromagnetic wave absorption

M. Ubaid-ur-Rehman Qureshi, Naveed Zafar Ali,\* Ubaid Ur Rehman, M. Nadeem and M. Aftab Rafiq

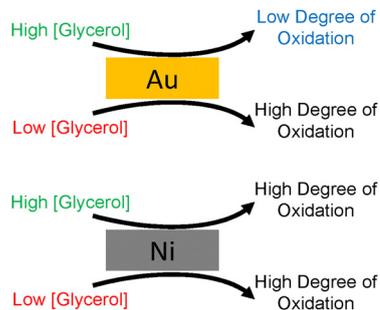
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### Improvement of electronic structure calculations for the interpretation of the emission spectrum for Nd<sup>III</sup> complexes

Yolimar Gil, María José Maldonado, Ricardo Costa de Santana, Andrés Vega, Pablo Fuentealba\* and Daniel Aravena\*

9855



### Effect of glycerol concentration on rate and product speciation for Ni and Au-based catalysts

Lauren C. Harris, Rachel N. Gaines, Qi Hua, Gavin S. Lindsay, James J. Griebler, Paul J. A. Kenis and Andrew A. Gewirth\*

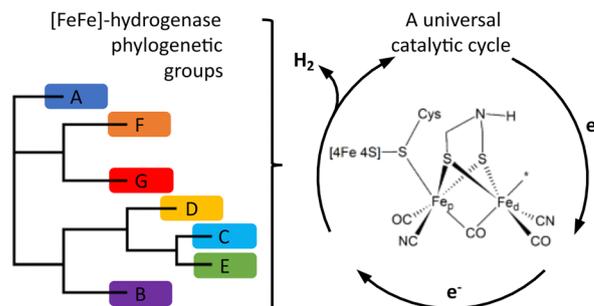


## RESEARCH PAPERS

9864

### Indications for a universal hydrogen catalysis mechanism in [FeFe]-hydrogenases of different phylogenetic groups

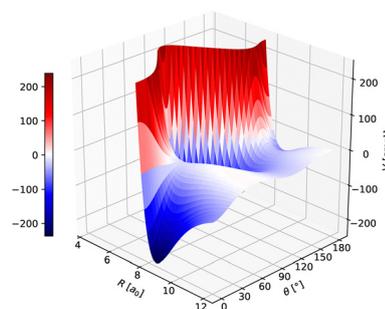
Moritz Senger,\* Conrad Schumann, Princess R. Cabotaje, Afridi Zamader, Ping Huang, Henrik Land and Gustav Berggren\*



9876

### Rotational (de-)excitation of CH<sub>3</sub>CN in collisions with H<sub>2</sub> on an accurate potential energy surface

M. Ben Khalifa,\* L. Wiesenfeld and J. Loreau\*



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### Hydrogen migration reactions *via* low internal energy pathways in aminobenzoic acid dications

Onni Veteläinen,\* Morsal Babayan, Lassi Pihlava, Abdul Rahman Abid, Antti Kivimäki, Edwin Kukk, Noelle Walsh, Samuli Urpelainen, Olle Björneholm, Marko Huttula, Matti Alatalo, Minna Patanen and Sergio Díaz-Tendero\*

