

## IN THIS ISSUE

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### Cover

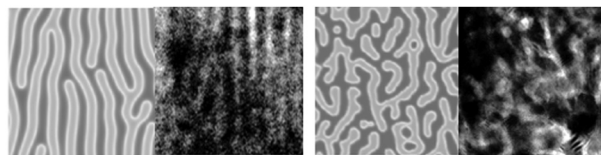
See Derrick Poe,  
Michael J. Servis *et al.*,  
pp. 14108–14121.  
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Michael Servis from  
*Phys. Chem. Chem. Phys.*,  
2024, 26, 14108.

## COMMUNICATION

14103

### Phase textures of metal–oxide nanocomposites self-orchestrated by atomic diffusions through precursor alloys

Nasrat Hannah Shudin, Ryuto Eguchi, Takeshi Fujita,\*  
Tomoharu Tokunaga, Ayako Hashimoto and Hideki Abe\*

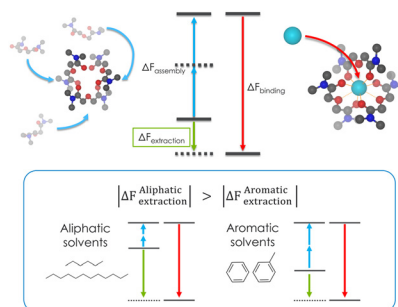


## RESEARCH PAPERS

14108

### Molecular-scale understanding of diluent effects on ligand assembly for metal ion separations

Derrick Poe,\* Soenke Seifert and Michael J. Servis\*



# RSC Applied Interfaces

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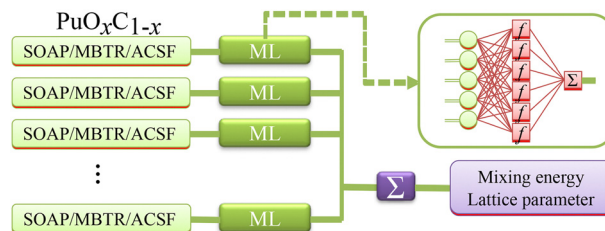
Fundamental questions  
Elemental answers

## RESEARCH PAPERS

14122

## Exploring thermodynamic stability of plutonium oxycarbide using a machine-learning scheme

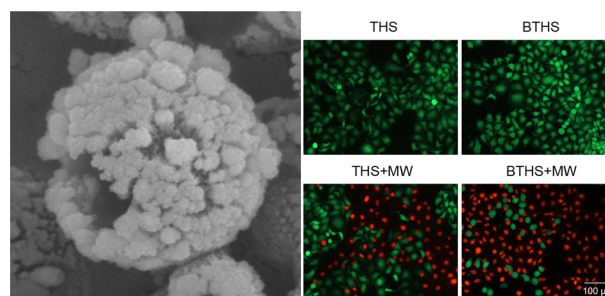
Ruizhi Qiu,\* Jun Tang, Jinfan Chen, Pengchuang Liu and Qi Wang\*



14131

Construction of  $\text{BaTiO}_3$ – $\text{TiO}_2$  hollow sphere heterojunctions for enhanced microwave dynamic therapy in cancer treatment

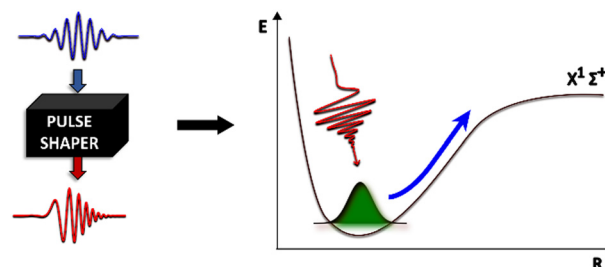
Yaodong Chen,\* Fangyu Cai, Yadong Liu, Wenwen Fan, Jingjie Wang, Guolin Yin, Jiayi Ren, Jingwei Cao, Yongming Fu\* and Jie Chen\*



14140

Dissociation of  $\text{HeH}^+$  in the electronic ground state using shaped mid-IR laser pulses

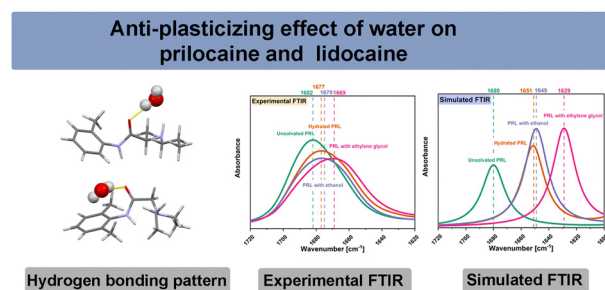
Kasper L. Effersø and Niels E. Henriksen



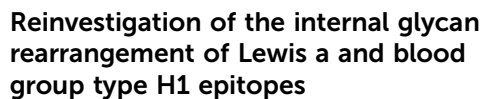
14149

## Anti-plasticizing effect of water on prilocaine and lidocaine – the role of the hydrogen bonding pattern

Xiaoyue Xu, Holger Grohgan\* and Thomas Rades







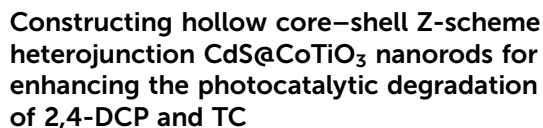
14171



14186



14194



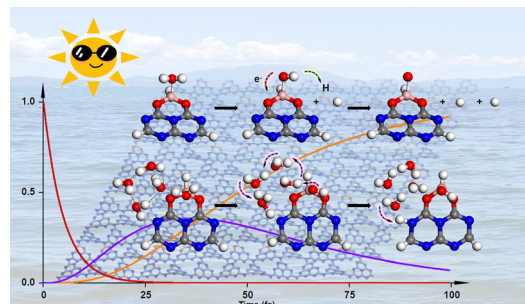
Jianhua Zheng,\* Yiming Gao, Bingbing Wang,  
Zhenping Guan, Guangming Yin,\* Heshan Zheng,  
Yong Li, Xiangyu Cao and Shunji Zheng

## RESEARCH PAPERS

14205

# Ultrafast hydrogen production in boron/oxygen-codoped graphitic carbon nitride revealed by nonadiabatic dynamics simulations

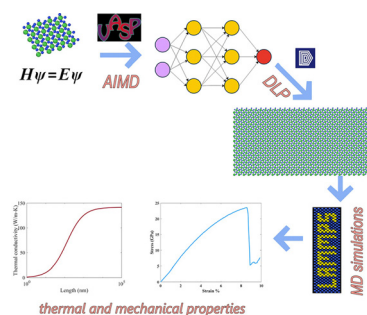
Huijuan Yang, Rongliang Wu, Wei Li and Jin Wen\*



14216

# Lattice thermal conductivity and mechanical properties of the single-layer penta-NiN<sub>2</sub> explored by a deep-learning interatomic potential

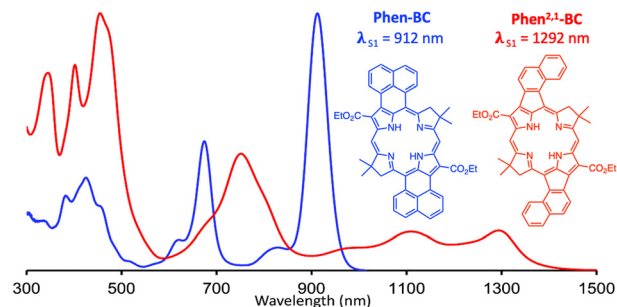
Pedram Mirchi, Christophe Adessi, Samy Merabia and Ali Rajabpour\*



14228

# Extension of nature's NIR-I chromophore into the NIR-II region

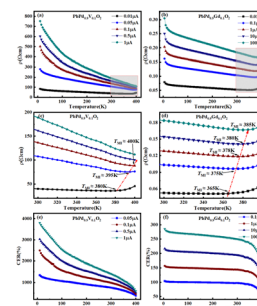
Kittipan Siwawannapong, James R. Diers, Nikki Cecil M. Magdaong, Phattananawee Nalaoh, Christine Kirmaier, Jonathan S. Lindsey,\* Dewey Holten\* and David F. Bocian\*



14244

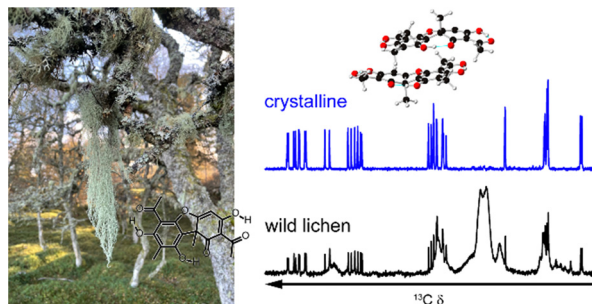
# Effects of V and Gd doping on novel positive colossal electroresistance and quantum transport in PbPdO<sub>2</sub> thin films with (002) preferred orientation

Hai Jia, Liqiang Zeng, Wenti Guo, Zhiya Lin, Jian-Min Zhang, Xiaohui Huang, Zhigao Huang\* and Shaoming Ying\*



## RESEARCH PAPERS

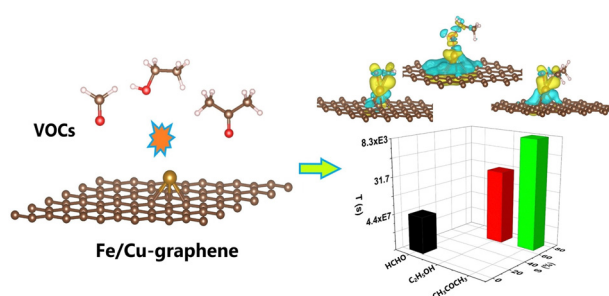
14256



## An NMR crystallographic characterisation of solid (+)-usnic acid

Daniel M. Dawson,\* Iain A. Smellie and Sharon E. Ashbrook\*

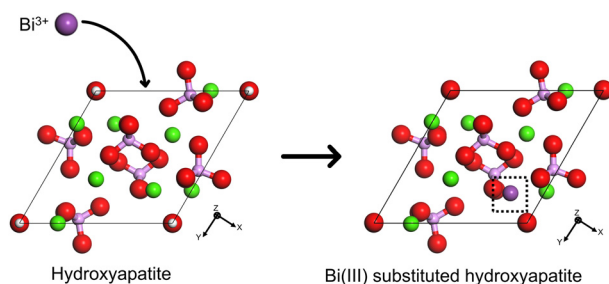
14265



## Theoretical insights into the adsorption and gas sensing performance of Fe/Cu-adsorbed graphene

Ngoc Tri Nguyen,\* Dai Q. Ho and Nguyen Tien Trung\*

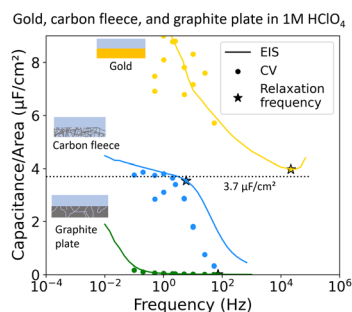
14277



## Site preference and local structural stability of Bi(III) substitution in hydroxyapatite using first-principles simulations

Gerardo Martin Quindoza, Yasuhiro Nakagawa, Hayato Laurence Mizuno, Yasutaka Anraku, Richard Espiritu and Toshiyuki Ikoma\*

14288



## How microstructures, oxide layers, and charge transfer reactions influence double layer capacitances. Part 1: impedance spectroscopy and cyclic voltammetry to estimate electrochemically active surface areas (ECSAs)

Maximilian Schalenbach,\* Victor Selmert, Ansgar Kretschmar, Luc Raijmakers, Yasin Emre Durmus, Hermann Tempel and Rüdiger-A. Eichel

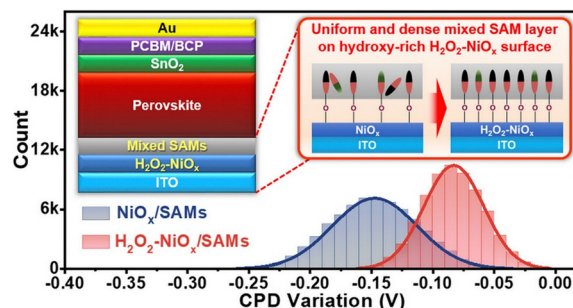


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14305

## A regulation strategy of self-assembly molecules for achieving efficient inverted perovskite solar cells

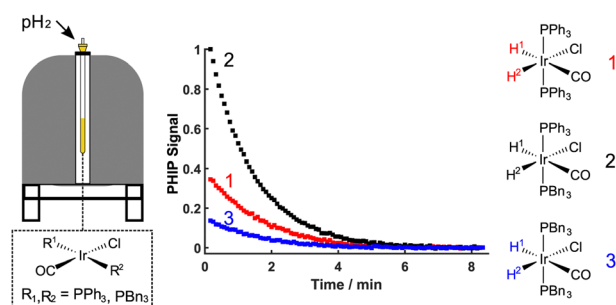
Pu-An Lin, Bo Yang, Changqing Lin, Zhenghui Fan, Yu Chen, Wenfeng Zhang, Bing Cai,\* Jie Sun,\* Xiaojia Zheng and Wen-Hua Zhang\*



14317

## Quantitative reaction monitoring using parahydrogen-enhanced benchtop NMR spectroscopy

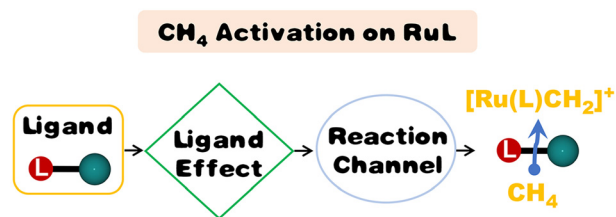
Alastair D. Robinson, Fraser Hill-Casey, Simon B. Duckett\* and Meghan E. Halse\*



14329

## Ligand effect on Ru-centered species toward methane activation

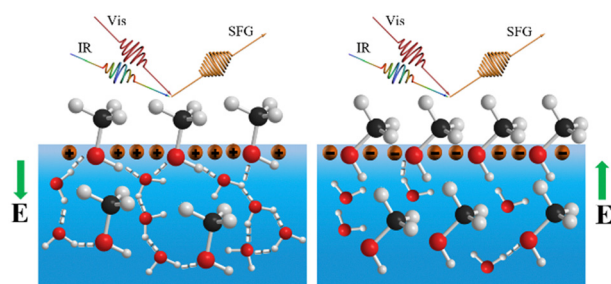
Mengdi Guo, Xiaonan Wu,\* Hechen Wu and Xiaoyan Sun\*



14336

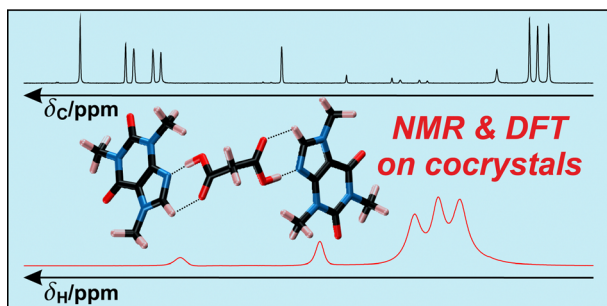
## Probing the adsorption configuration of methanol at a charged air/aqueous interface using nonlinear spectroscopy

Caihe Liu, Xujin Qin, Changhui Yu, Yuan Guo and Zhen Zhang\*



## RESEARCH PAPERS

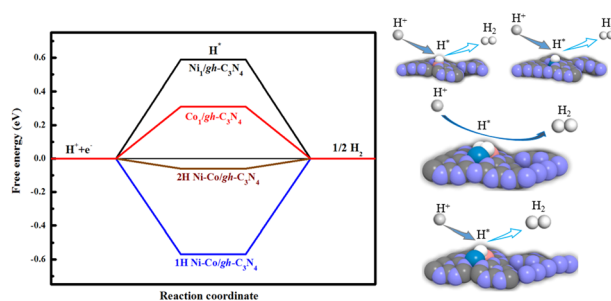
14345



$^1\text{H}$  and  $^{13}\text{C}$  chemical shift–structure effects in anhydrous  $\beta$ -caffeine and four caffeine–diacid cocrystals probed by solid-state NMR experiments and DFT calculations

Debashis Majhi, Baltzar Stevansson, Tra Mi Nguyen and Mattias Edén\*

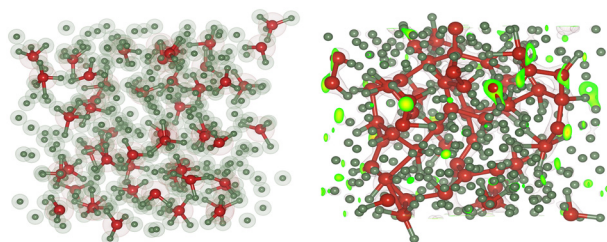
14364



Graphitic carbon nitride supported Ni–Co dual-atom catalysts beyond  $\text{Ni}_1(\text{Co}_1)$  single-atom catalysts for hydrogen production: a density functional theory study

Yue He, Furui Chen and Gang Zhou\*

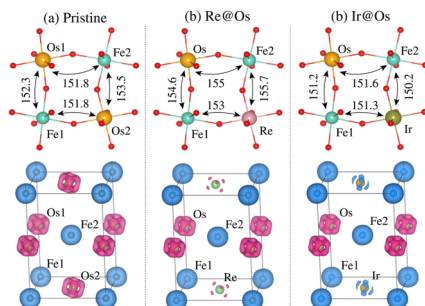
14374



Mixture of hydrogen and methane under planetary interior conditions

Argha Jyoti Roy,\* Armin Bergemann, Mandy Bethkenhagen and Ronald Redmer

14384



Re/Ir@Os-doping induced insulator-to-metal transition in Mott-insulator  $\text{Ca}_2\text{FeOsO}_6$ : octahedral distortion effects

S. Nazir



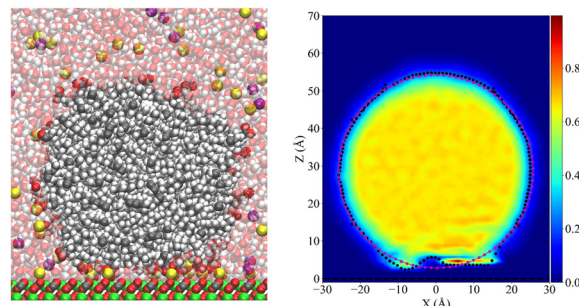


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14393

**Salinity and pH effects on water–oil–calcite interfaces by using molecular dynamics**

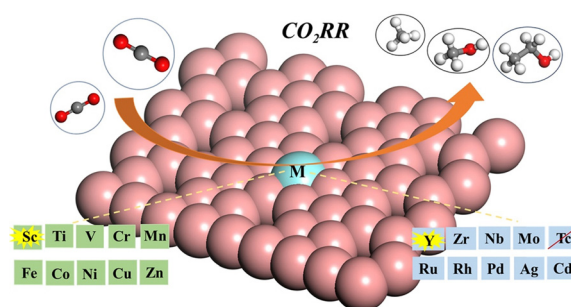
Anderson Arboleda-Lamus, Leonardo Muñoz-Rugeles, Jorge M. del Campo, Nicolas Santos-Santos, Julio Pérez and Enrique Mejía-Ospino\*



14407

**Theoretical study of transition metal-doped  $\beta_{12}$  borophene as a new single-atom catalyst for carbon dioxide electroreduction**

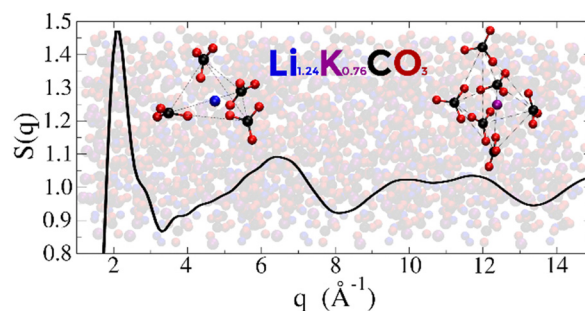
Hongjie Huang, Mingyao Chen, Rongxin Zhang, Yuxuan Ding, Hong Huang, Zhangfeng Shen, Lingchang Jiang, Zhigang Ge, Hongtao Jiang, Minhong Xu,\* Yangang Wang\* and Yongyong Cao\*



14420

**Structure and dynamics of  $\text{Li}_{1.24}\text{K}_{0.76}\text{CO}_3$  molten carbonate electrolyte from molecular simulations with explicit polarization**

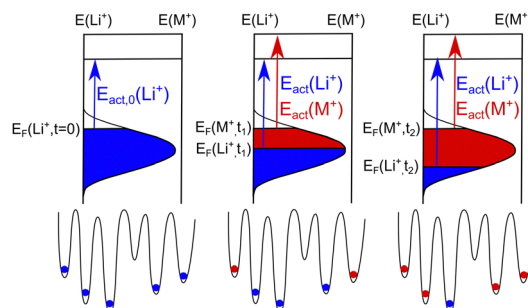
Francesco Sessa, Massimiliano Della Pietra, Simone Mataloni, Ana B. Muñoz-García and Michele Pavone\*



14430

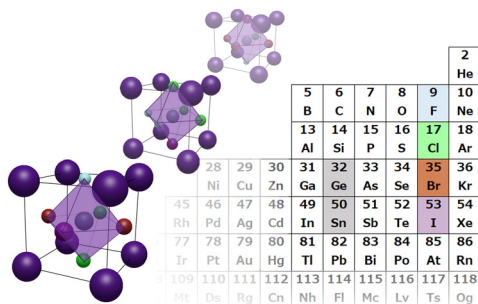
**Manifestation of site energy landscapes for ion transport in borate glasses**

Victor H. Gunawan, Martin Schäfer and Karl-Michael Weitzel\*



## RESEARCH PAPERS

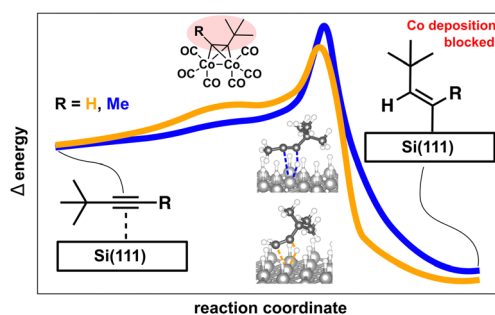
14440



### High-throughput calculation for the screening of formamidinium halide perovskite for solar cells

Tomoya Tashiro,\* Hajime Suzuki and Keisuke Takahashi\*

14448



### Mechanistic study of the atomic layer deposition of cobalt: a combined mass spectrometric and computational approach

Sofia Donnecke,\* Mathias Paul, Peter J. H. Williams, Serena Chan, Veronica Tse, Jigyasa Sachdeva, Allen G. Oliver, J. Scott McIndoe\* and Irina Paci\*

