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### Cover

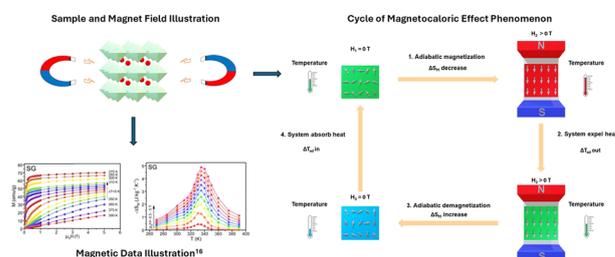
See Stefan Fuchs and Bernhard Dick, pp. 14514–14528. Image reproduced by permission of Bernhard Dick and Roger-Jan Kutta from Phys. Chem. Chem. Phys., 2024, 26, 14514.

## REVIEW

14476

### The magnetocaloric effect properties for potential applications of magnetic refrigerator technology: a review

Phahul Zhemas Zul Nehan, Okvarahireka Vitayaya, Dicky Rezky Munazat, Maykel T. E. Manawan, Darminto Darminto and Budhy Kurniawan\*

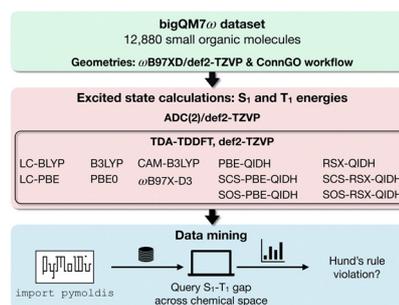


## COMMUNICATION

14505

### Resilience of Hund's rule in the chemical space of small organic molecules

Atreyye Majumdar and Raghunathan Ramakrishnan\*



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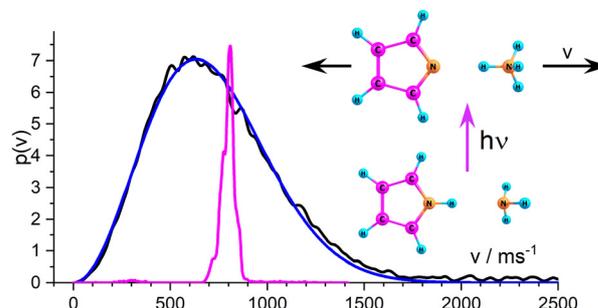
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## RESEARCH PAPERS

14514

## Photodissociation of deuterated pyrrole–ammonia clusters: H-atom transfer or electron coupled proton transfer?

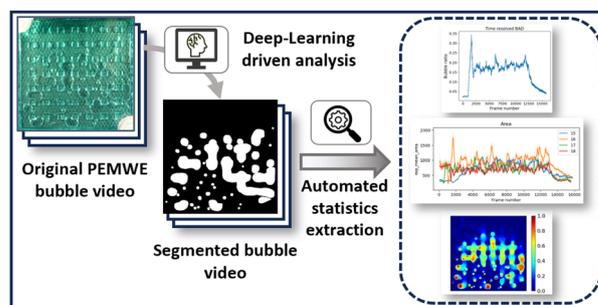
Stefan Fuchs and Bernhard Dick\*



14529

## Deep learning-enhanced characterization of bubble dynamics in proton exchange membrane water electrolyzers

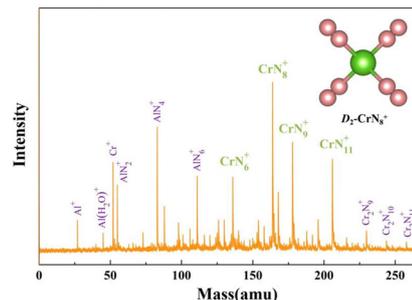
André Colliard-Granero, Keusra A. Gompou, Christian Rodenbücher, Kouroush Malek, Michael H. Eikerling and Mohammad J. Eslamibidgoli\*



14538

## Geometries and stabilities of chromium doped nitrogen clusters: mass spectrometry and density functional theory studies

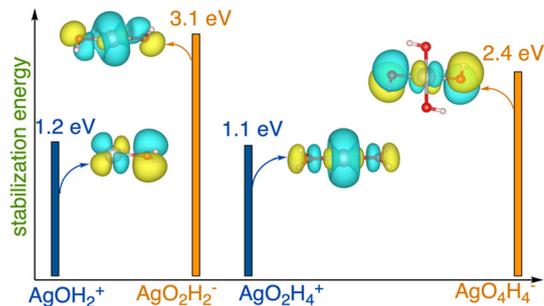
Zaifu Jiang, Peixin Fu, Meicheng Chen, Chen Chen, Bole Chen, Wei Dai, Kewei Ding\* and Cheng Lu\*



14547

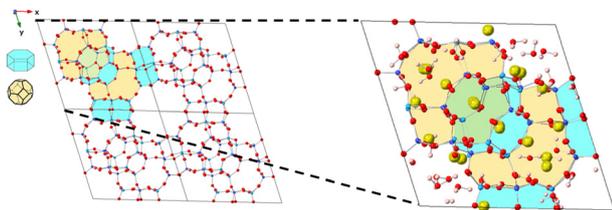
Electronic properties and collision cross sections of  $\text{AgO}_k\text{H}_m^\pm$  ( $k, m = 1-4$ ) aerosol ionic clusters

Mohsen Doust Mohammadi, Somnath Bhowmick\*, Anne Maisser, Andreas Schmidt-Ott and George Biskos\*



## RESEARCH PAPERS

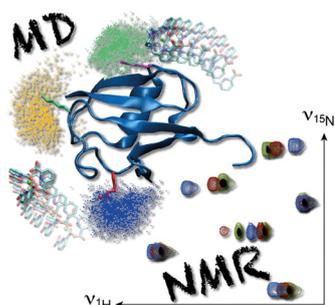
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### Incorporating solvent effects in DFT: insights from cation exchange in faujasites

An T. Ta, Ayoub Daouli, R. Seaton Ullberg, Eric Fonseca, Vanessa Proust, Agnès Grandjean, Richard G. Hennig, Hans-Conrad zur Loye, Michael Badawi\* and Simon R. Phillpot\*

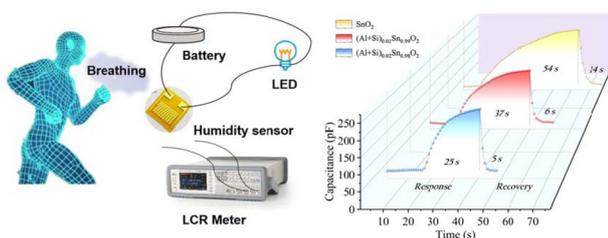
14573



### One touch is all it takes: the supramolecular interaction between ubiquitin and lanthanide complexes revisited by paramagnetic NMR and molecular dynamics

Karen Dos Santos, Alessio Bartocci, Natacha Gillet, Sandrine Denis-Quanquin, Amandine Roux, Eugene Lin, Zeren Xu, Raphael Finizola, Pauline Chedozeau, Xi Chen, Cédric Caradeuc, Mathieu Baudin, Gildas Bertho, François Riobé, Olivier Maury, Elise Dumont\* and Nicolas Giraud\*

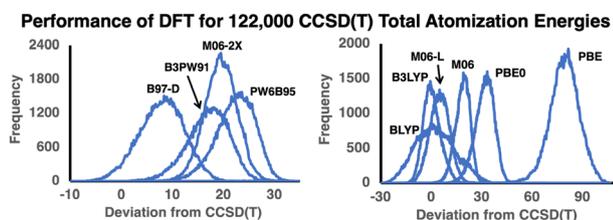
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### Investigation on acceptor–donor co-doped $\text{SnO}_2$ nanoparticles enriched with oxygen vacancies: a capacitive humidity sensor for respiration detection

Yuchuan Ding, Yong Chen and MaoHua Wang\*

14594



### Big data benchmarking: how do DFT methods across the rungs of Jacob's ladder perform for a dataset of 122k CCSD(T) total atomization energies?

Amir Karton

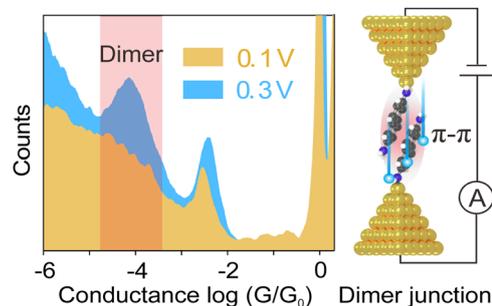


## RESEARCH PAPERS

14607

Regulation of  $\pi$ - $\pi$  interactions between single aromatic molecules by bias voltage

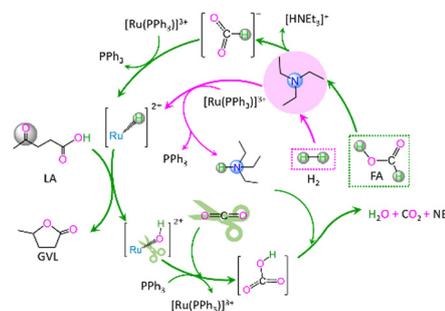
Xiaona Xu, Keqiang Jia, Qiang Qi, Guangjun Tian\* and Dong Xiang\*



14613

Mechanism of  $\text{CO}_2$  in promoting the hydrogenation of levulinic acid to  $\gamma$ -valerolactone catalyzed by  $\text{RuCl}_3$  in aqueous solution

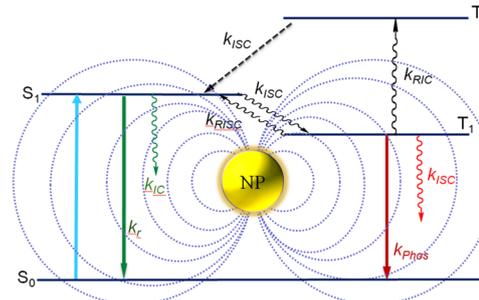
Han-Yun Min, Jin-Shan Xiong, Ting-Hao Liu, Shuai Fu, Chang-Wei Hu and Hua-Qing Yang\*



14624

## Molecular phosphorescence enhancement by the plasmon field of metal nanoparticles

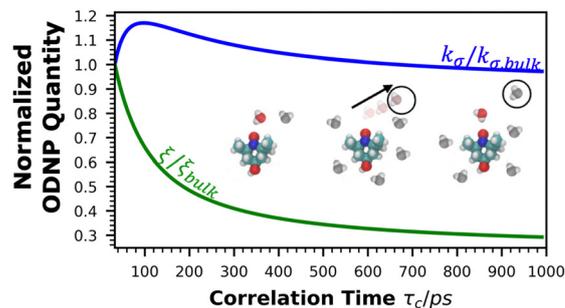
Niyazbek Kh. Ibrayev,\* Rashid R. Valiev,\* Evgeniya V. Seliverstova, Evgeniya P. Menshova, Rinat T. Nasibullin and Dage Sundholm



14637

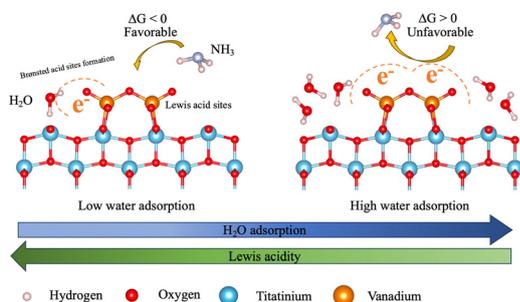
## Computation of Overhauser dynamic nuclear polarization processes reveals fundamental correlation between water dynamics, structure, and solvent restructuring entropy

Dennis C. Robinson Brown, Thomas R. Webber, Thomas M. Casey, John Franck, M. Scott Shell and Songi Han\*



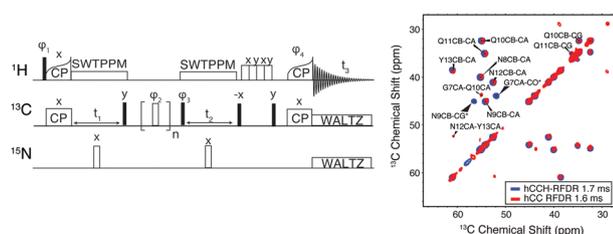
## RESEARCH PAPERS

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Theoretical insight into H<sub>2</sub>O impact on V<sub>2</sub>O<sub>5</sub>/TiO<sub>2</sub> catalysts for selective catalytic reduction of NO<sub>x</sub>

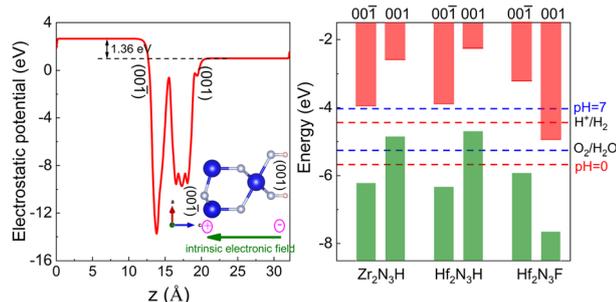
Boyu Wu, Shengen Zhang,\* Mingtian Huang, Shengyang Zhang, Bo Liu and Bolin Zhang\*

14664

Structural characterization of E22G Aβ<sub>1-42</sub> fibrils via <sup>1</sup>H detected MAS NMR

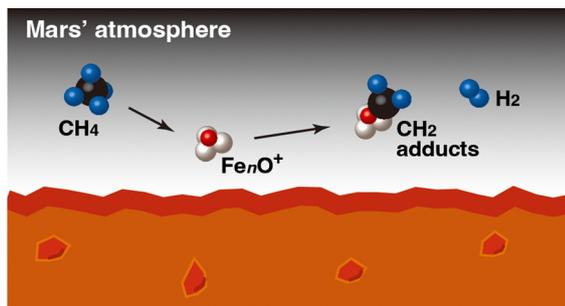
Natalie C. Golota, Brian Michael, Edward P. Saliba, Sara Linse and Robert G. Griffin\*

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Rational design of 2D Janus *P3m1* M<sub>2</sub>N<sub>3</sub> (M = Cu, Zr, and Hf) and their surface-functionalized derivatives: ferromagnetic, piezoelectric, and photocatalytic properties

Heng Zhang, Frédéric Guégan, Junjie Wang\* and Gilles Frapper\*

14684



## Reaction of size-selected iron-oxide cluster cations with methane: a model study of rapid methane loss in Mars' atmosphere

Masashi Arakawa,\* Satoshi Kono, Yasuhito Sekine and Akira Terasaki\*

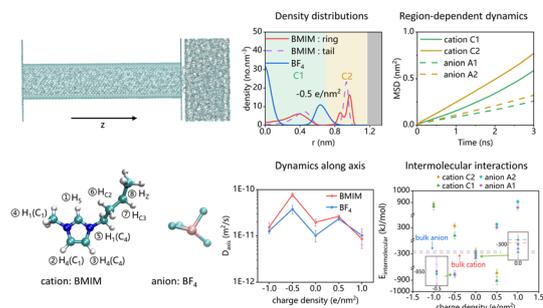


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14691

## Molecular insights into the nanoconfinement effect on the structure and dynamics of ionic liquids in carbon nanotubes

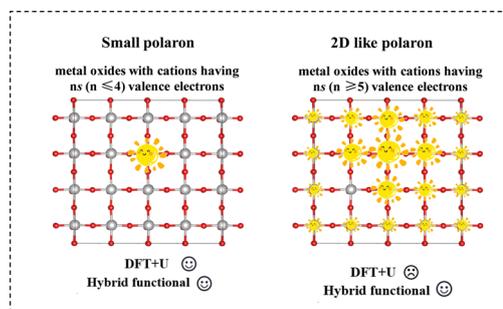
Hao-Qian Liu, Yong-Lei Wang and Bin Li\*



14705

## s valence electrons in cations of metal oxides serving as descriptors for electron and hole polarons

Junyan Tao and Taifeng Liu\*



14713

## Fast formation of anode-free Li-metal batteries by pulsed current

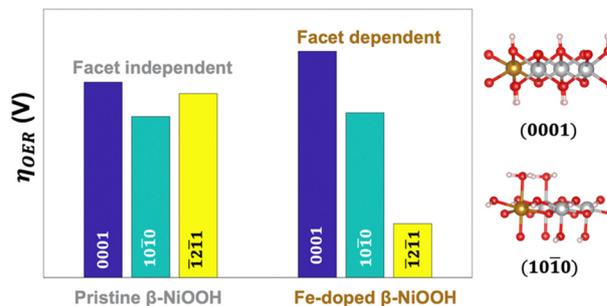
Katarina Cicvarić,\* Sebastian Pohlmann, Bojing Zhang, Fuzhan Rahmanian, Leon Merker, Miran Gaberšček and Helge Sören Stein\*



14721

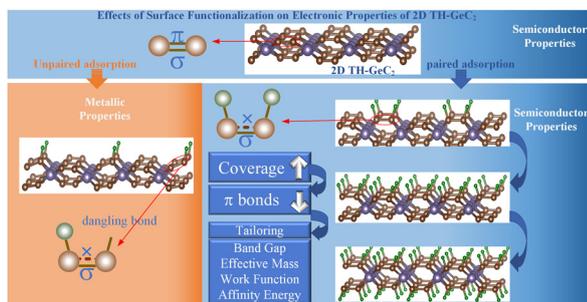
Strongly facet-dependent activity of iron-doped  $\beta$ -nickel oxyhydroxide for the oxygen evolution reaction

Ananth Govind Rajan,\* John Mark P. Martirez and Emily A. Carter\*



## RESEARCH PAPERS

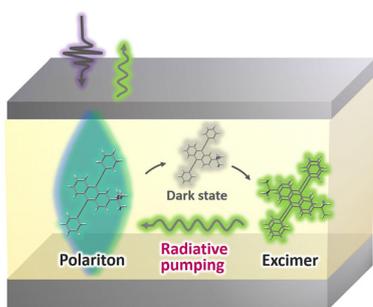
14734



### Effect and mechanism analysis of surface hydrogenation and fluorination on the electronic properties of th-GeC<sub>2</sub>

Guihong Luo, Ying Yang,\* Yajie Zhu, Xihong Peng and Li He

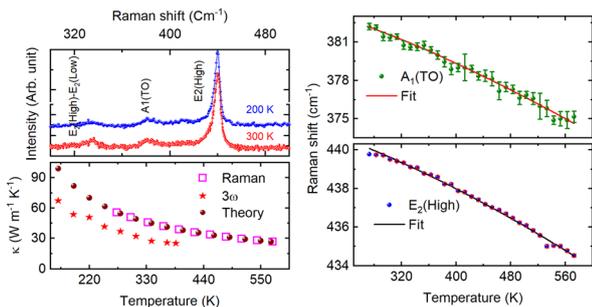
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### Radiative pumping in a strongly coupled microcavity filled with a neat molecular film showing excimer emission

Yoichi Sasaki,\* Kyriacos Georgiou, Shuangqing Wang, David G. Bossanyi, Rahul Jayaprakash, Nobuhiro Yanai, Nobuo Kimizuka, David G. Lidzey, Andrew J. Musser and Jenny Clark\*

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### Lattice thermal conductivity of ZnO: experimental and theoretical studies

Satyasiban Dash and Prahallad Padhan\*

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### An eminent approach towards next generation solvents for sustainable packaging and stability of enzymes: a comprehensive study of ionic liquid and deep eutectic solvent mixtures

Urooj Fatima, Nirmala Deenadayalu and Pannuru Venkatesu\*

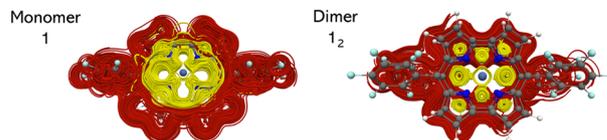


## RESEARCH PAPERS

14777

### Changing aromatic properties through stacking: the face-to-face dimer of Ni(II) bis(pentafluorophenyl)norcorrole

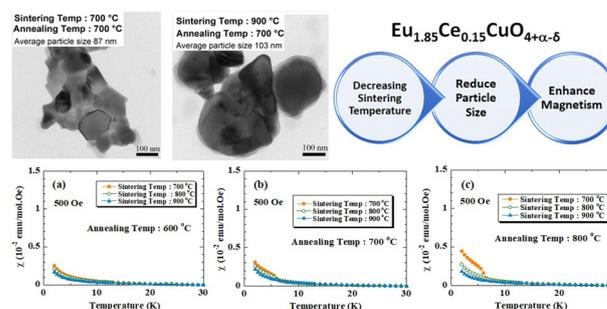
Qian Wang, Dage Sundholm,\* Jürgen Gauss, Tommaso Nottoli, Filippo Lipparini, Shota Kino, Shusaku Ukai, Norihito Fukui and Hiroshi Shinokubo



14787

### Enhancement of magnetism by tailoring synthesis conditions in electron-doped superconducting nanoparticles

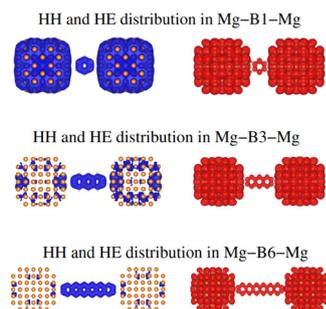
Muhammad Fadhil Falhan, Suci Winarsih, Rosaldi Pratama, Muhammad Abdan Syakuur, Utami Widayiswari, Anita Eka Putri and Risdiana\*



14796

### Hot carrier creation in a nanoparticle dimer-molecule composite

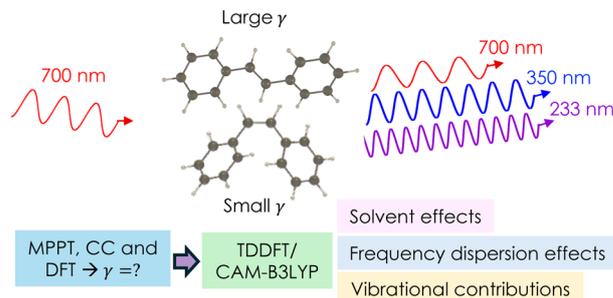
Junais Habeeb Mokkath



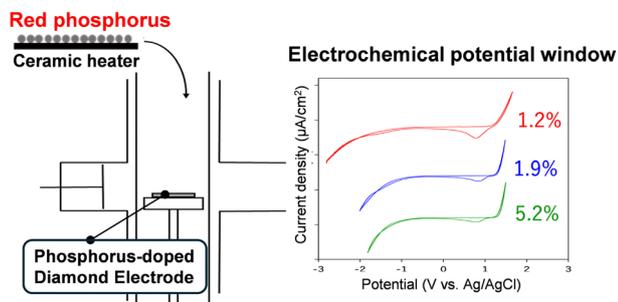
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### On the third-order nonlinear optical responses of *cis* and *trans* stilbenes – a quantum chemistry investigation

Komlanvi Sèvi Kaka, Frédéric Castet and Benoît Champagne\*



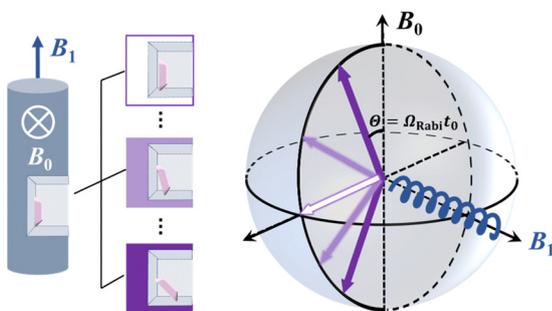
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### Fabrication of polycrystalline phosphorus-doped diamond electrodes from red phosphorus

Tomokiyo Moriguchi, Mai Tomisaki, Susumu Sato, Jin Nakamura, Hideaki Yamada and Yasuaki Einaga\*

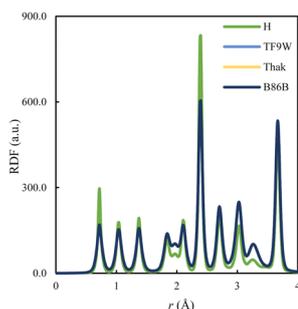
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### Angular-resolved Rabi oscillations of orthorhombic spins in a Co(II) molecular qubit

Yi-Qiu Liao, You-Chao Liu, Yi-Han Wang, Peng-Xiang Fu, Yi Xie, Song Gao, Ye-Xin Wang,\* Zheng Liu\* and Shang-Da Jiang\*

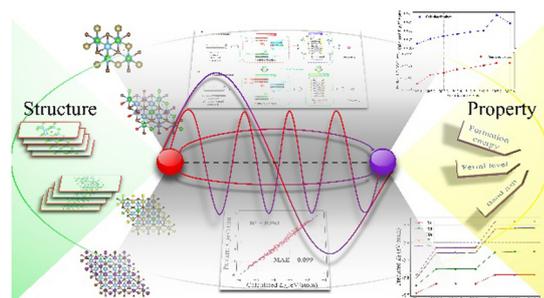
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### Reaction rate constant: a theoretical description from local temperature

Saba Valatoon and Mojtaba Alipour\*

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### Leveraging an all-fixed transfer framework to predict the interpretable formation energy of MXenes with hybrid terminals

Zihao Song, Xiaobin Niu and Haiyuan Chen\*

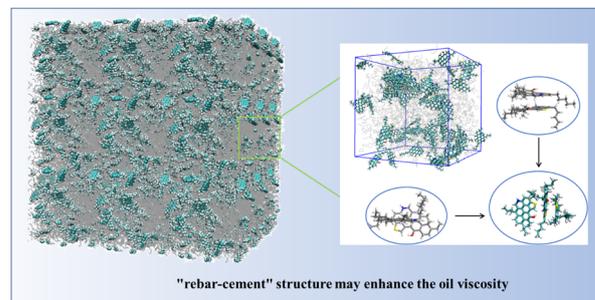


## RESEARCH PAPERS

14857

### New insight into the role of the self-assembly of heteroatom compounds in heavy oil viscosity enhancement

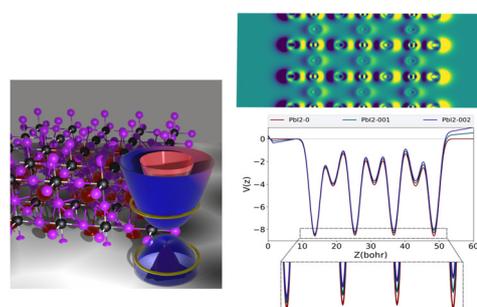
Jichao Fang, Bingyu Ji, Xueyu Wang,\* Shideng Yuan and Haiying Yu\*



14866

### Layer-dependent spin texture and origins of Rashba splitting quenching in the 2D CsPbI<sub>3</sub> perovskite

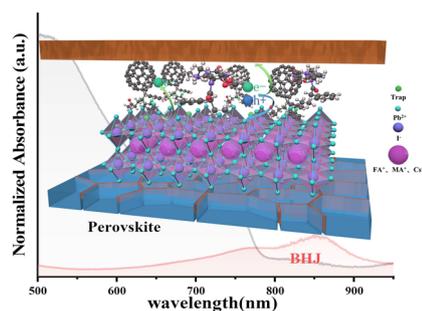
Safieh Nazari\* and Yavar T. Azar



14874

### Revealing the impact of thermal annealing on the perovskite/organic bulk heterojunction interface in photovoltaic devices

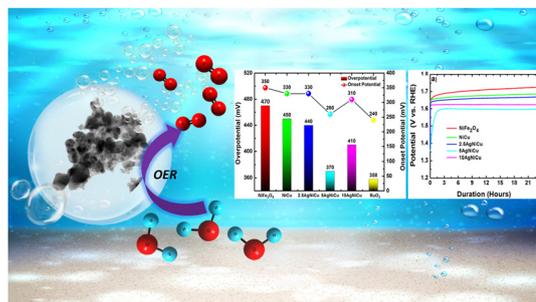
Peng Chen, Xinyuan Ma, Zhiyu Wang, Nan Yang, Jianwen Luo, Ke Chen,\* Pengyi Liu, Weiguang Xie and Qin Hu\*



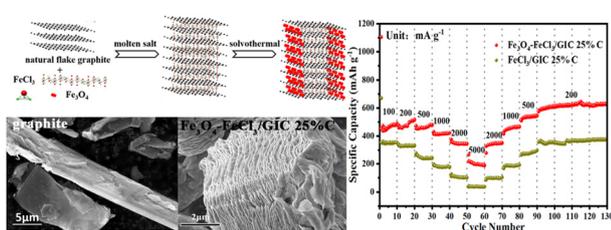
14883

### Silver nanoparticle-decorated NiFe<sub>2</sub>O<sub>4</sub>/CuWO<sub>4</sub> heterostructure electrocatalyst for oxygen evolution reactions

Uttam Kumar, Kumar Sanket, Rupesh Mandal, Arup Kumar De, Anshu Shrivastava, Shantanu K. Behera\* and Indrajit Sinha\*



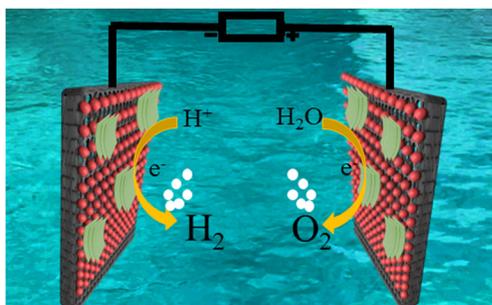
14898



### Fe<sub>3</sub>O<sub>4</sub>-modified FeCl<sub>3</sub>/graphite intercalation compound confinement architecture for unleashing the high-performance anode potential of lithium-ion batteries

Kai Zhou, Baiyu Guo, Jun Ma, Siyu Cui, Yuying Bao, Tao Wang,\* Hailong Qiu\* and Di Jin\*

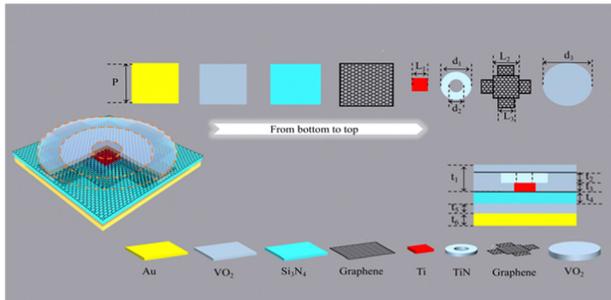
14908



### A high-performance electrocatalyst via graphitic carbon nitride nanosheet-decorated bimetallic phosphide for alkaline water electrolysis

Zehra Kayış and Duygu Akyüz\*

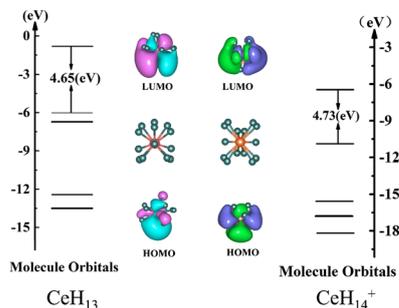
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### A tunable ultra-broadband and ultra-high sensitivity far-infrared metamaterial absorber based on VO<sub>2</sub> and graphene

Hengli Feng, Hongyan Meng, Guan Wang, Jia Liu, Xin Zhang, Meichen Li, Shuang Yang, Yang Jia, Hanmo Du, Yang Gao and Yachen Gao\*

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### Exploring the structure and hydrogen storage capacity of CeH<sub>n</sub><sup>0/+</sup> clusters

H. H. Zhao, S. J. Huang, X. S. Li,\* W. W. Yu, Y. W. Fu, Y. Liu and H. Y. Wang

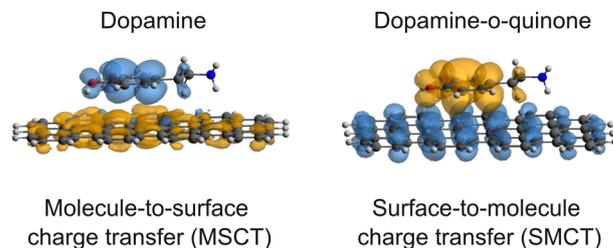


## RESEARCH PAPERS

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**Theoretical insights into dopamine photochemistry adsorbed on graphene-type nanostructures**

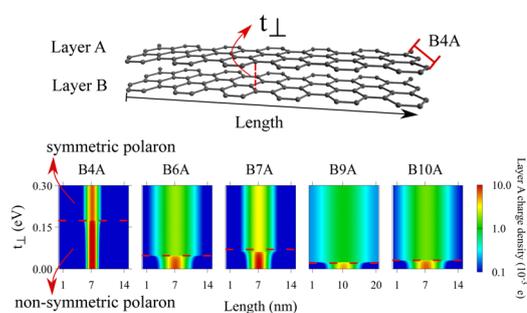
Alex-Adrian Farcaş and Attila Bende\*



14948

**Width effects on bilayer graphene nanoribbon polarons**

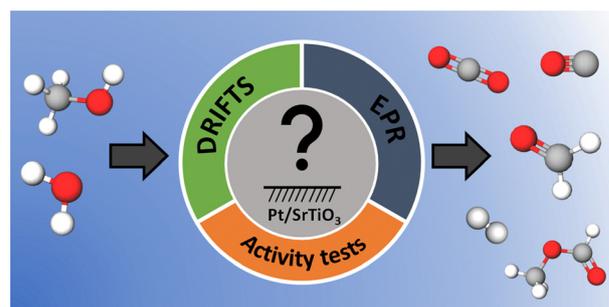
André Lima Logrado, Tiago de Sousa Araújo Cassiano, William Ferreira da Cunha, Ricardo Gargano, Geraldo Magela e Silva and Pedro Henrique de Oliveira Neto\*



14960

**Mechanistic understanding of the thermal-assisted photocatalytic oxidation of methanol-to-formaldehyde with water vapor over Pt/SrTiO<sub>3</sub>**

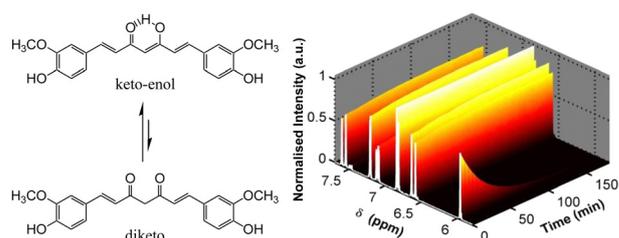
Michel Deitermann, Takuma Sato, Yannik Haver, Alexander Schnegg, Martin Muhler and Bastian Timo Mei\*



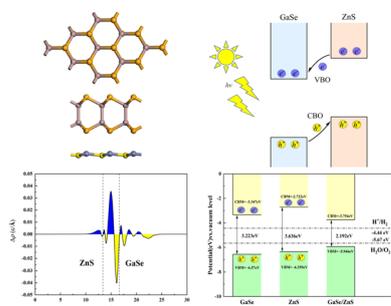
14970

**Time-resolved keto–enol tautomerization of the medicinal pigment curcumin**

Mandy H. M. Leung, Matthew A. Addicoat, Stephen F. Lincoln, Gregory F. Metha and Tak W. Kee\*



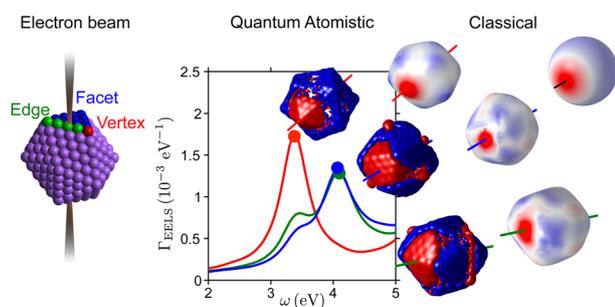
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### Carrier mobility and optical properties of a type-II GaSe/ZnS heterostructure as a photocatalyst: a first-principles study

Yongqiang Ma, Aida Bao,\* Xin Guo\* and Jie Wang

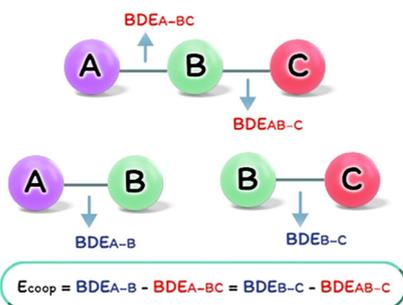
14991



### Footprints of atomic-scale features in plasmonic nanoparticles as revealed by electron energy loss spectroscopy

Mattin Urbieto,\* Marc Barbry, Peter Koval, Alberto Rivacoba, Daniel Sánchez-Portal, Javier Aizpurua and Nerea Zabala\*

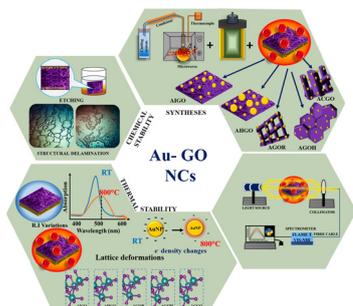
15005



### Can we quantitatively evaluate the mutual impacts of intramolecular metal–ligand bonds the same as intermolecular noncovalent bonds?

Samaneh Sanei Movafagh and Sadegh Salehzadeh\*

15018



### Chemically engineered plasmonic Au–gallium oxide nanocomposites for harsh environment applications: an investigation into thermal and chemical robustness

L. Keerthana and Gnanaprakash Dharmalingam\*



15032

## On the nature of sub-THz continuum absorption in CO<sub>2</sub> gas, its mixture with Ar, and in pure water vapor

T. A. Galanina, A. O. Koroleva, I. S. Amerkhanov,  
E. A. Serov, M. A. Koshelev, M. Yu. Tretyakov,\*  
D. N. Chistikov, A. A. Finenko and A. A. Vigin

