Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PCCP

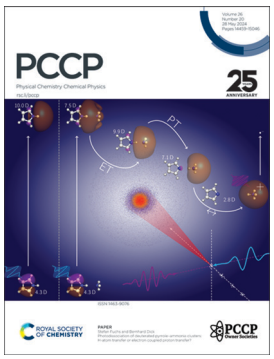
Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(20) 14459–15046 (2024)



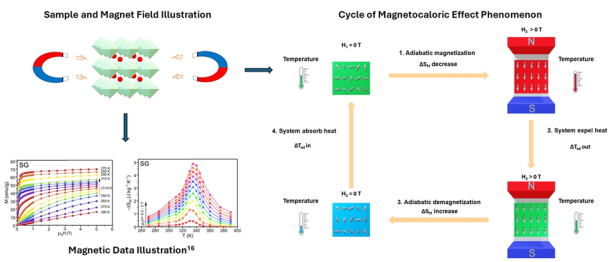
Cover
See Stefan Fuchs and Bernhard Dick, pp. 14514–14528. Image reproduced by permission of Bernhard Dick and Roger-Jan Kutta from Phys. *Chem. Chem. Phys.*, 2024, **26**, 14514.

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*

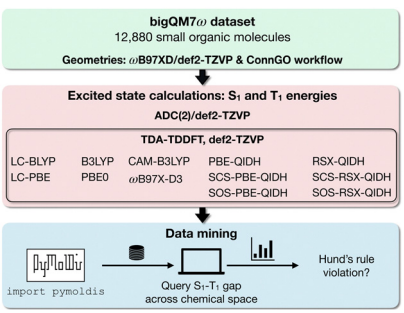


COMMUNICATION

14505

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

Atreyee Majumdar and Raghunathan Ramakrishnan*



View Article Online

Industrial Chemistry & Materials

GOLD OPEN ACCESS

Focus on industrial chemistry
Advance material innovations
Highlight interdisciplinary feature

Innovative.
Interdisciplinary.
Problem solving

APCs currently waived

Learn more about ICM
Submit your high-quality article

@IndChemMater

@IndChemMater

rsc.li/icm

ROYAL SOCIETY OF CHEMISTRY

Industrial Chemistry & Materials

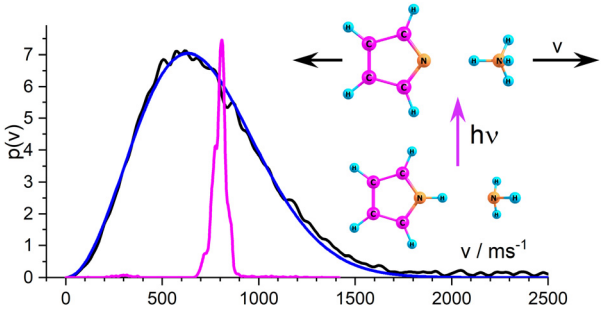
Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

14514

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

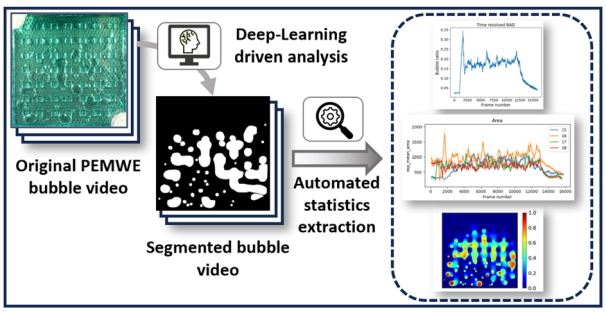
Stefan Fuchs and Bernhard Dick*



14529

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

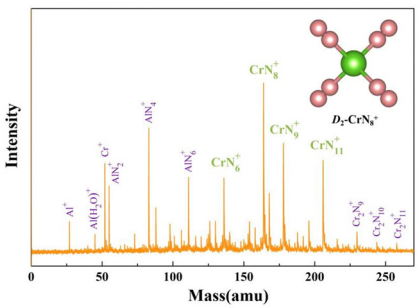
André Colliard-Granero, Keusra A. Gompou, Christian Rodenbücher, Kourosh Malek, Michael H. Eikerling and Mohammad J. Eslamibidgoli*



14538

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

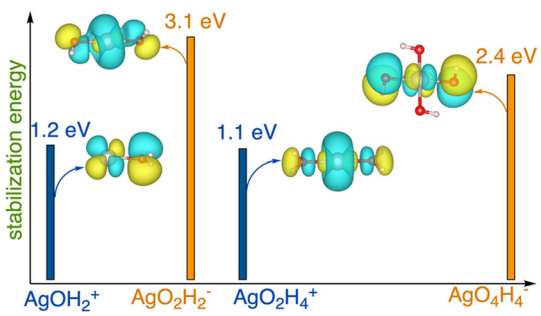
Zaifu Jiang, Peixin Fu, Meicheng Chen, Chen Chen, Bole Chen, Wei Dai, Kewei Ding* and Cheng Lu*



14547

Electronic properties and collision cross sections of $AgO_kH_m^{\pm}$ (k, m = 1–4) aerosol ionic clusters

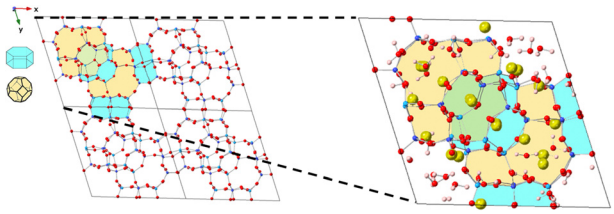
Mohsen Doust Mohammadi, Somnath Bhowmick,* Anne Maisser, Andreas Schmidt-Ott and George Biskos*



Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

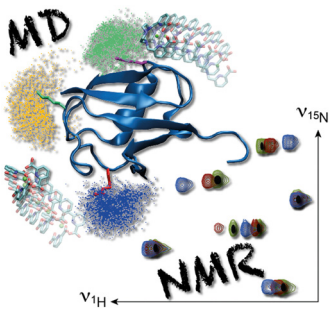
14561



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*

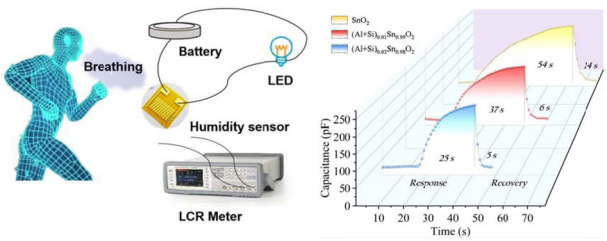
14573



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*

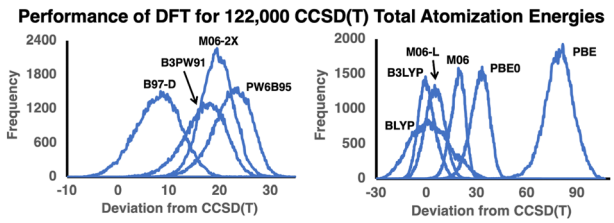
14582



Investigation on acceptor–donor co-doped 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

This journal is © the Owner Societies 2024

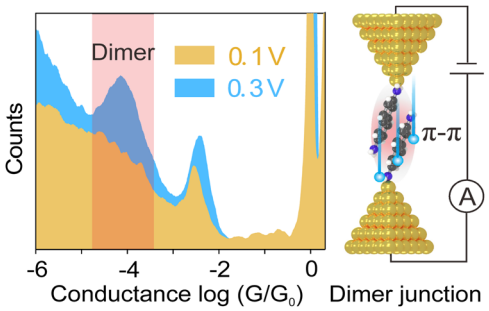
Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

14607

Regulation of π–π interactions between single aromatic molecules by bias voltage

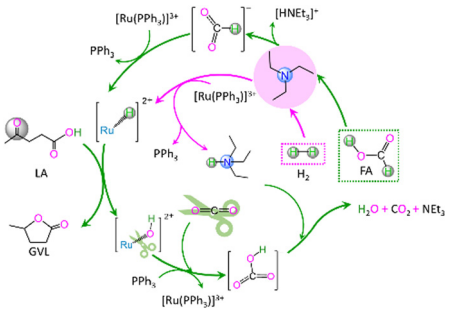
Xiaona Xu, Keqiang Jia, Qiang Qi, Guangjun Tian* and Dong Xiang*



14613

Mechanism of CO_2 in promoting the hydrogenation of levulinic acid to γ-valerolactone catalyzed by $RuCl_3$ in aqueous solution

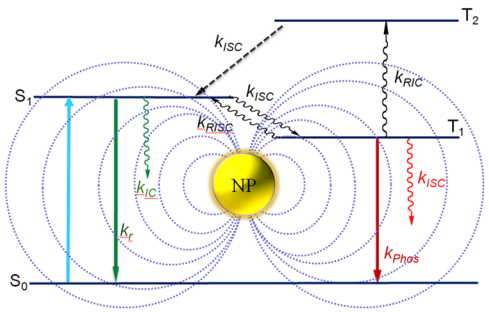
Han-Yun Min, Jin-Shan Xiong, Ting-Hao Liu, Shuai Fu, Chang-Wei Hu and Hua-Qing Yang*



14624

Molecular phosphorescence enhancement by the plasmon field of metal nanoparticles

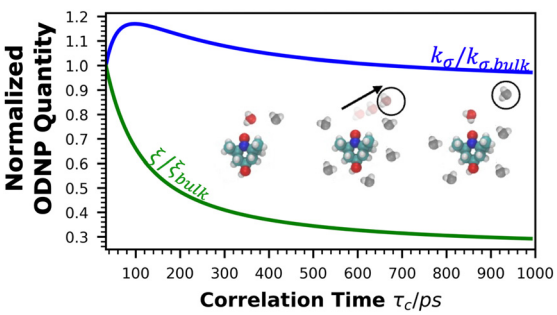
Niyazbek Kh. Ibrayev,* Rashid R. Valiev,* Evgeniya V. Seliverstova, Evgeniya P. Menshova, Rinat T. Nasibullin and Dage Sundholm



14637

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

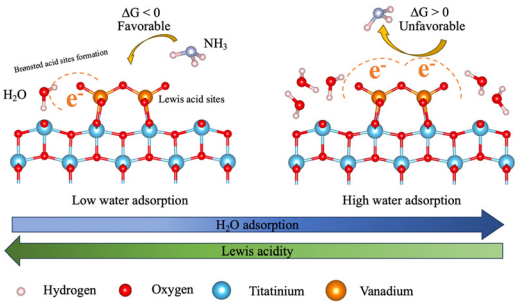
Dennis C. Robinson Brown, Thomas R. Webber, Thomas M. Casey, John Franck, M. Scott Shell and Songi Han*



Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

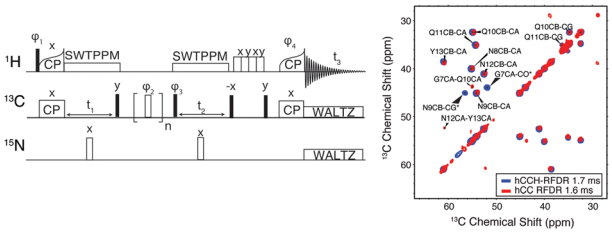
14651



Theoretical insight into H_2O impact on V_2O_5/TiO_2 catalysts for selective catalytic reduction of NO_x

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

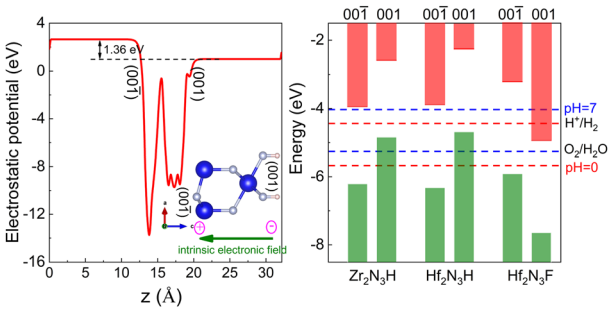
14664



Structural characterization of E22G $A\beta_{1-42}$ fibrils *via* ^1H detected MAS NMR

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

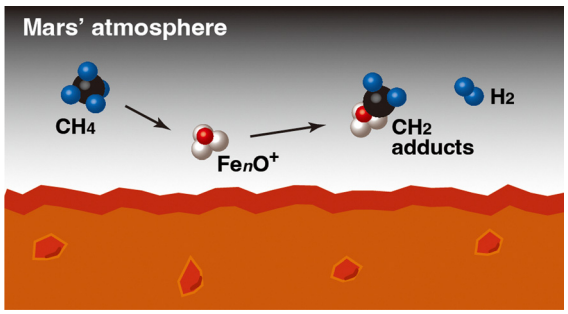
14675



Rational design of 2D Janus *P*3*m*1 M_2N_3 (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*

This journal is © the Owner Societies 2024

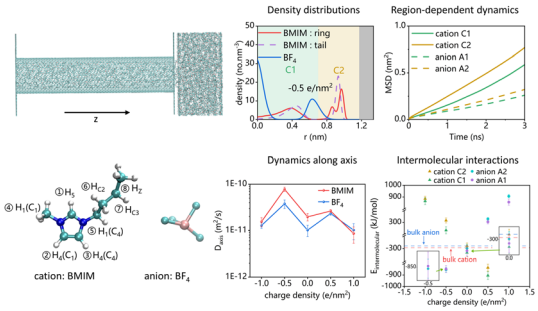
Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

14691

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

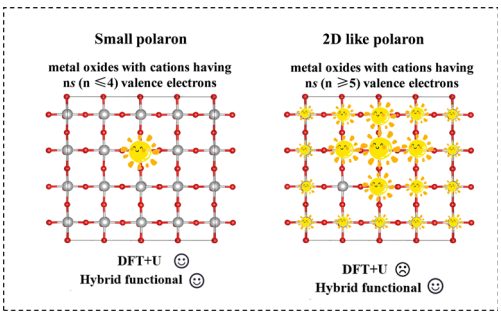
Hao-Qian Liu, Yong-Lei Wang and Bin Li*



14705

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

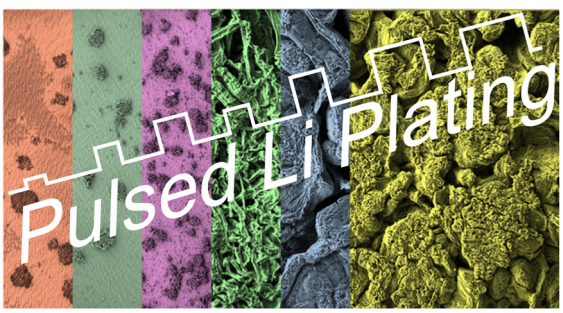
Junyan Tao and Taifeng Liu*



14713

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

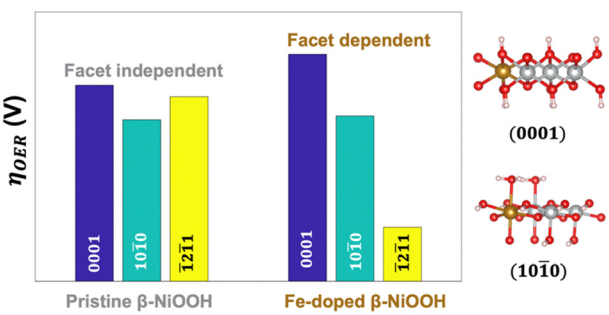
Katarina Cicvarić,* Sebastian Pohlmann, Bojing Zhang, Fuzhan Rahmanian, Leon Merker, Miran Gaberšček and Helge Sören Stein*



14721

Strongly facet-dependent activity of iron-doped β-nickel oxyhydroxide for the oxygen evolution reaction

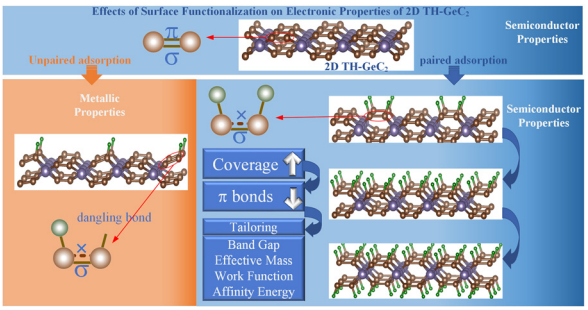
Ananth Govind Rajan,* John Mark P. Martirez and Emily A. Carter*



Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

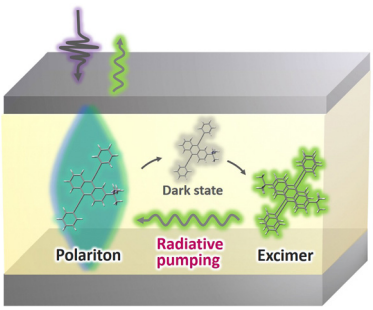
14734



Effect and mechanism analysis of surface hydrogenation and fluorination on the electronic properties of th-GeC_2

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

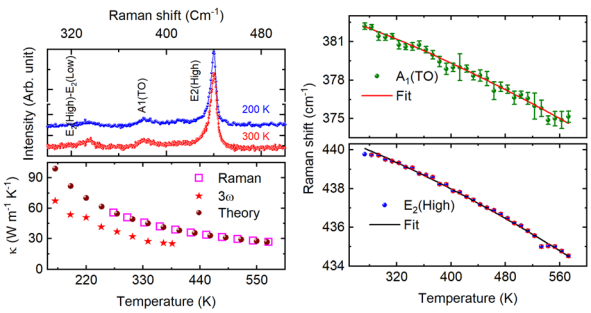
14745



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*

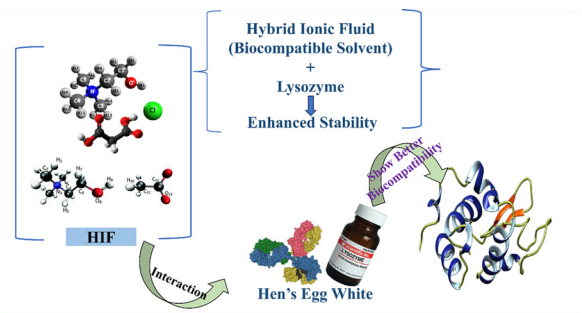
14754



Lattice thermal conductivity of ZnO: experimental and theoretical studies

Satyasiban Dash and Prahallad Padhan*

14766



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*

This journal is © the Owner Societies 2024

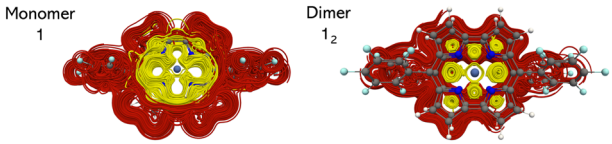
Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

14777

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

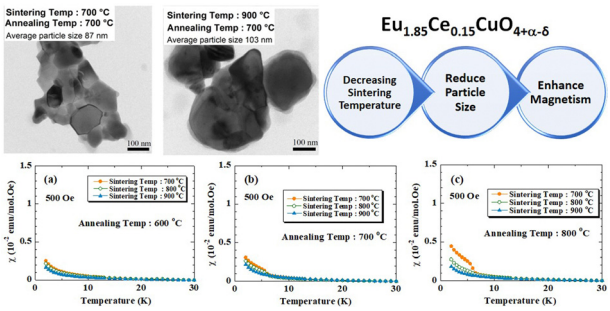
Qian Wang, Dage Sundholm,* Jürgen Gauss, Tommaso Nottoli, Filippo Lipparini, Shota Kino, Shusaku Ukai, Norihito Fukui and Hiroshi Shinokubo



14787

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

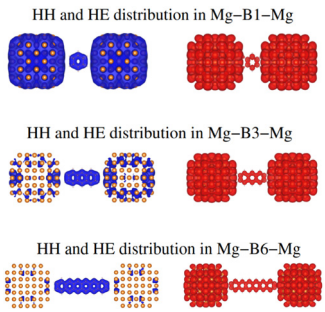
Muhammad Fadhil Falhan, Suci Winarsih, Rosaldi Pratama, Muhammad Abdan Syakuur, Utami Widyaiswari, Anita Eka Putri and Risdiana*



14796

Hot carrier creation in a nanoparticle dimer-molecule composite

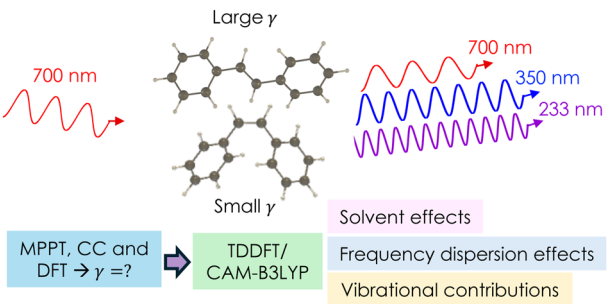
Junais Habeeb Mokkath



14808

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

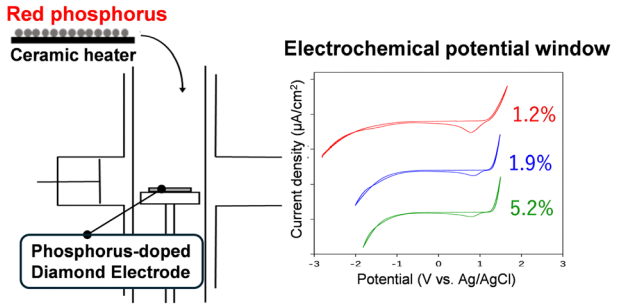
Komlanvi Sèvi Kaka, Frédéric Castet and Benoît Champagne*



Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

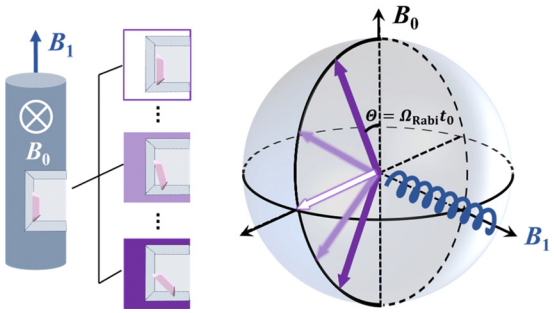
14825



Fabrication of polycrystalline phosphorus-doped diamond electrodes from red phosphorus

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

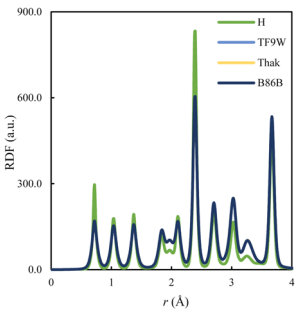
14832



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*

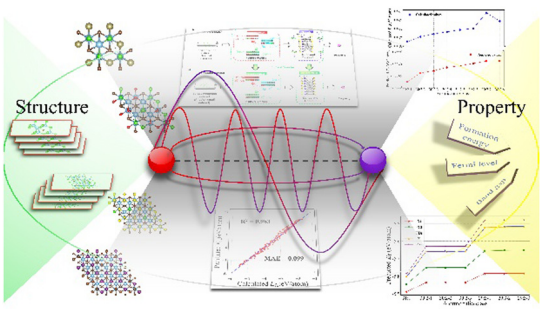
14839



Reaction rate constant: a theoretical description from local temperature

Saba Valatoon and Mojtaba Alipour*

14847



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

Zihao Song, Xiaobin Niu and Haiyuan Chen*

This journal is © the Owner Societies 2024

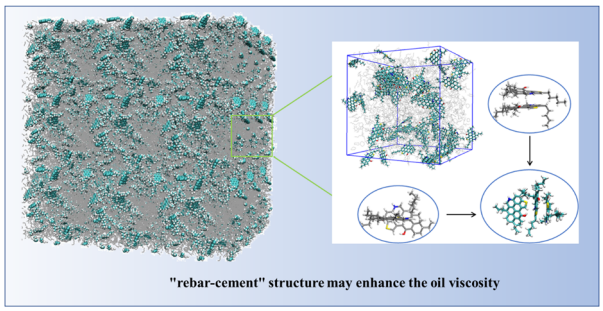
Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

14857

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

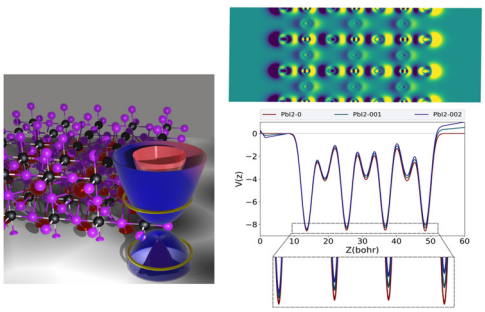
Jichao Fang, Bingyu Ji, Xueyu Wang,* Shideng Yuan and Haiying Yu*



14866

Layer-dependent spin texture and origins of Rashba splitting quenching in the 2D $CsPbI_3$ perovskite

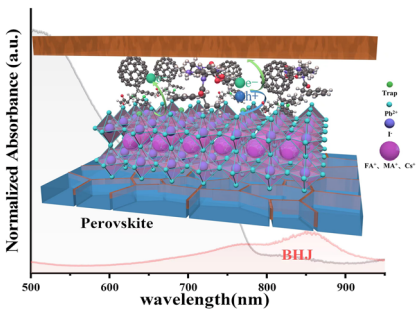
Safieh Nazari* and Yavar T. Azar



14874

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

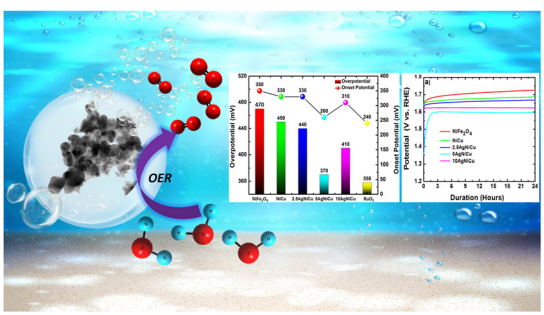
Peng Chen, Xinyuan Ma, Zhiyu Wang, Nan Yang, Jianwen Luo, Ke Chen,* Pengyi Liu, Weiguang Xie and Qin Hu*



14883

Silver nanoparticle-decorated $NiFe_2O_4/CuWO_4$ heterostructure electrocatalyst for oxygen evolution reactions

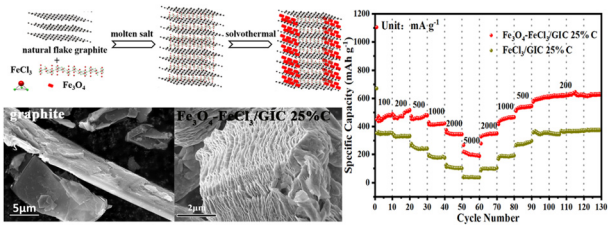
Uttam Kumar, Kumar Sanket, Rupesh Mandal, Arup Kumar De, Anshu Shrivastava, Shantanu K. Behera* and Indrajit Sinha*



Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

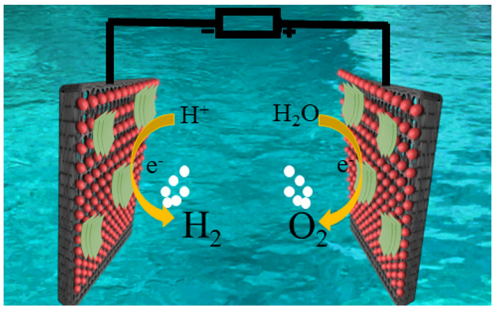
14898



Fe_3O_4-modified $FeCl_3$/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*

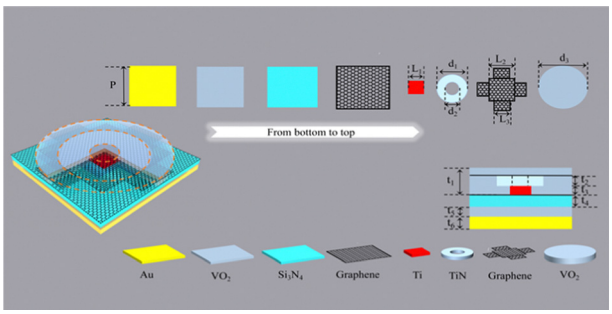
14908



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

Zehra Kayış and Duygu Akyüz*

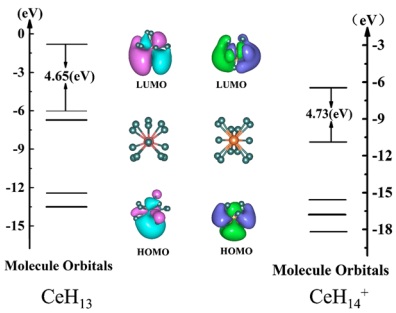
14919



A tunable ultra-broadband and ultra-high sensitivity far-infrared metamaterial absorber based on VO_2 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*

14930



Exploring the structure and hydrogen storage capacity of $CeH_n^{0/+}$ clusters

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

This journal is © the Owner Societies 2024

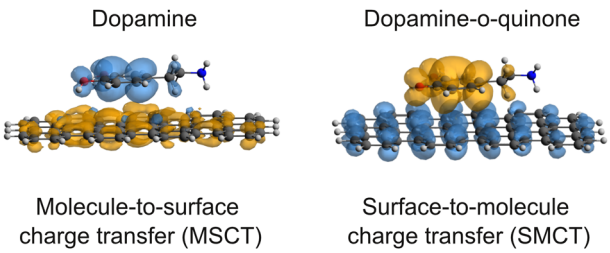
Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

14937

Theoretical insights into dopamine photochemistry adsorbed on graphene-type nanostructures

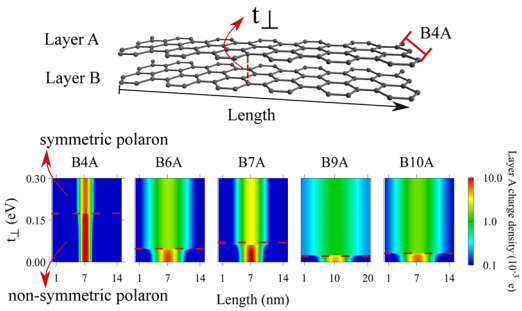
Alex-Adrian Farcaş and Attila Bende*



14948

Width effects on bilayer graphene nanoribbon polarons

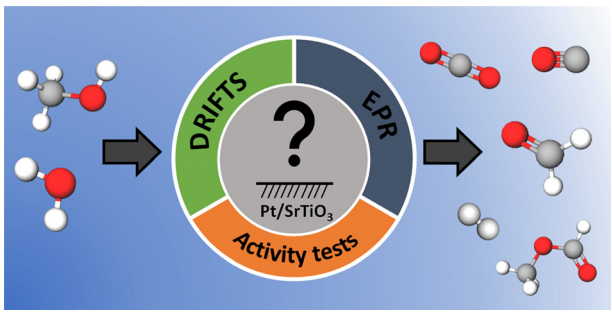
André Lima Logrado, Tiago de Sousa Araújo Cassiano, Wiliam Ferreira da Cunha, Ricardo Gargano, Geraldo Magela e Silva and Pedro Henrique de Oliveira Neto*



14960

Mechanistic understanding of the thermal-assisted photocatalytic oxidation of methanol-to-formaldehyde with water vapor over Pt/SrTiO$_3$

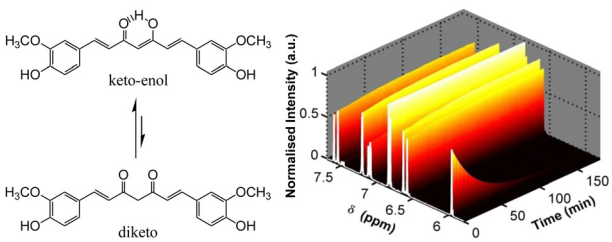
Michel Deitermann, Takuma Sato, Yannik Haver, Alexander Schnegg, Martin Muhler and Bastian Timo Mei*



14970

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

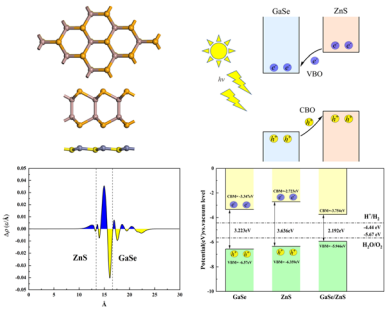
Mandy H. M. Leung, Matthew A. Addicoat, Stephen F. Lincoln, Gregory F. Metha and Tak W. Kee*



Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

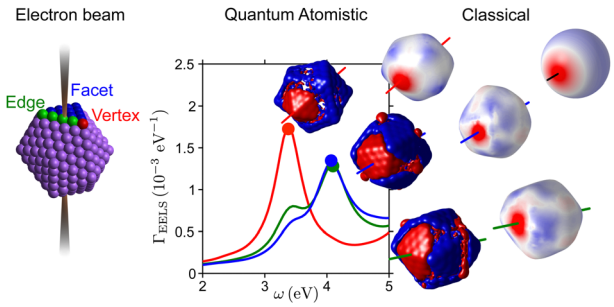
14980



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

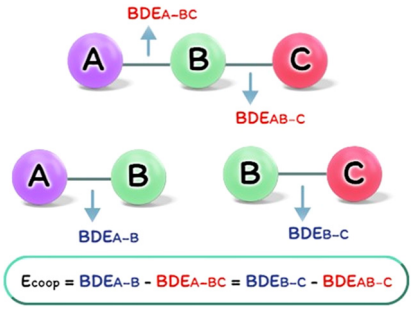
14991



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

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

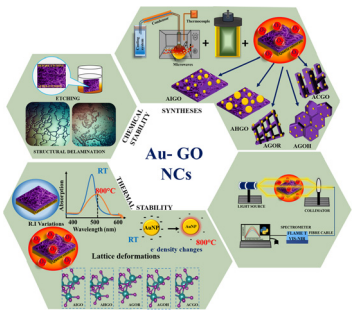
15005



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

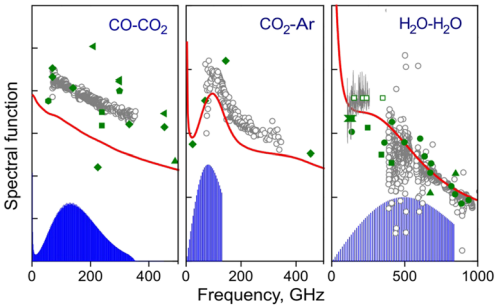
L. Keerthana and Gnanaprakash Dharmalingam*

This journal is © the Owner Societies 2024

15032

On the nature of sub-THz continuum absorption in CO_2 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. Vigasin



Open Access Article. Published on 22 May 2024. Downloaded on 3/14/2026 8:50:57 PM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.