Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PCCP

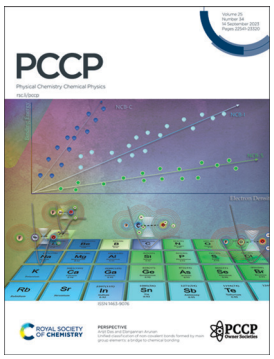
Physical Chemistry Chemical Physics – An international journal

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 25(34) 22541–23320 (2023)



Cover
See Arijit Das and Elangannan Arunan, pp. 22583–22594. Image reproduced by permission of Arijit Das and Elangannan Arunan from *Phys. Chem. Chem. Phys.*, 2023, **25**, 22583.

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

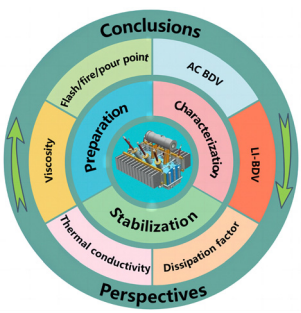
Aurora E. Clark,* Pavlo O. Dral,* Isaac Tamblyn* and Olexandr Isayev*

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*



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

Editorial Staff

Executive Editor
Michael A. Rowan

Deputy Editor
Vikki Pritchard

Development Editors
Bee Hockin, Andrea Carolina Ojeda Porras

Editorial Production Manager
Gisela Scott

Senior Publishing Editor
Robin Brabham

Publisher
Jeanne Andres

Publishing Editors
Catherine Au, Isobel Darlington, Konoya Das, Alexandre Dumon, Amy Lucas, Kieran Nicholson, Rini Prakash, Charlotte Pugsley, Hugh Ryan

Publishing Assistant
Robert Griffiths

Editorial Assistant
Daphne Houston

For queries about submitted papers, please contact Gisela Scott, Editorial Production Manager, in the first instance. E-mail: **pccp@rsc.org**

For pre-submission queries, please contact Michael A. Rowan, Executive Editor.
Email: **pccp-rsc@rsc.org**

PCCP (electronic lSSN 1463-9084) is published 48 times a year by the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.

All orders, with cheques made payable to the Royal Society of Chemistry, should be sent to the Royal Society of Chemistry Order Department, Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, CB4 0WF, UK.
Tel +44 (0)1223 432398; E-mail: **orders@rsc.org**

2023 Annual (electronic) subscription price: £4448; US$7835. Customers in Canada will be subject to a surcharge to cover GST. Customers in the EU subscribing to the electronic version only will be charged VAT.

If you take an institutional subscription to any Royal Society of Chemistry journal you are entitled to free, site-wide web access to that journal. You can arrange access via Internet Protocol (IP) address at **www.rsc.org/ip**

Customers should make payments by cheque in sterling payable on a UK clearing bank or in US dollars payable on a US clearing bank.

Whilst this material has been produced with all due care, the Royal Society of Chemistry cannot be held responsible or liable for its accuracy and completeness, nor for any consequences arising from any errors or the use of the information contained in this publication. The publication of advertisements does not constitute any endorsement by the Royal Society of Chemistry or Authors of any products advertised. The views and opinions advanced by contributors do not necessarily reflect those of the Royal Society of Chemistry which shall not be liable for any resulting loss or damage arising as a result of reliance upon this material. The Royal Society of Chemistry is a charity, registered in England and Wales, Number 207890, and a company incorporated in England by Royal Charter (Registered No. RC000524), registered office: Burlington House, Piccadilly, London W1J 0BA, UK. Telephone: +44 (0) 207 4378 6556.

Advertisement sales:
Tel +44 (0) 1223 432246;
Fax +44 (0) 1223 426017;
E-mail **advertising@rsc.org**

For marketing opportunities relating to this journal, contact **marketing@rsc.org**

ROYAL SOCIETY OF CHEMISTRY

PCCP

Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

PCCP is an international journal for the publication of original research papers, Communications and Perspective articles in the areas of physical chemistry, chemical physics and biophysical chemistry.

Owner Societies

Canadian Society for Chemistry
Deutsche Bunsen-Gesellschaft für Physikalische Chemie
Institute of Chemistry of Ireland
Israel Chemical Society
Kemisk Forenin
Koninklijke Nederlandse Chemische Vereniging
Korean Chemical Society
New Zealand Institute of Chemistry
Norsk Kjemisk Selskap
Österreichische Physikalische Gesellschaft
Polskie Towarzystwo Chemiczne
Real Sociedad Española de Química
Royal Australian Chemical Institute Incorporated
Royal Society of Chemistry
Società Chimica Italiana
Suomen Kemian Seura – Kemiska Sällskapet I Finland
Svenska Kemisamfundet
Swiss Chemical Society
Türkiye Kimya Derneği

Honorary Board

G Ertl, Berlin, Germany
B Feringa, University of Groningen, Netherlands
S W Hell, Max Planck Institute for Biophysical Chemistry, Germany
J Jortner, Tel Aviv, Israel
M Karplus, Harvard University, USA
K Kohse- Hoeinghaus, Universitaet Bielefeld, Germany
Y T Lee, Academia Sinica, Taiwan
W H Miller, Berkeley, USA
E Neher, Max Planck Institute for Biophysical Chemistry, Germany
J Polanyi, Toronto, Canada
H Schwarz, Technische Universität Berlin, Germany
J P Simons, University of Oxford, UK
G A Somorjai, University of California, Berkeley, USA
J Troe, GWDG, Germany
R N Zare, Stanford, USA

Editorial Board

B Albinsson, Chalmers University of Technology, Sweden
L Bañares, Universidad Complutense de Madrid, Spain
M Curri, University of Bari, Italy
C Daniel, Institute of Chemistry, University of Strasbourg, France
K Gordon, University of Otago, New Zealand
H Kondoh, Keio University, Japan
A Krylov, University of Southern California, USA
P Maiti, Indian Institute of Science, India
R Naaman, Weizmann Institute of Science, Israel
A Rijs, Vrije Universiteit Amsterdam, The Netherlands (Chair)
H Schaefer lll, University of Georgia, USA (Deputy Chair)
I Tamblyn, University of Ottawa, Canada
Y Xu, University of Alberta, Canada
J Zhang, New York University Shanghai, China

Advisory Board

C Adamo, ENSCP - Chimie ParisTech, France
H Ågren, KTH Royal Institute of Technology, Sweden
K Ariga, National Institute for Materials Science, Japan
P Ayers, McMaster University, Canada
A Ajayaghosh, CSIR-National Institute for Interdisciplinary Science and Technology (NIIST), India
P Baglioni, University of Florence, Italy
V Barone, Scuola Normale Superiore di Pisa, Italy
M Biczysko, Shanghai University, China
E Bieske, University of Melbourne, Australia
J Biteen, University of Michigan, USA
D Casanova, Donostia International Physics Center, Spain
P Casavecchia, University of Perugia, Italy
O Christiansen, University of Aarhus, Denmark
G A Cisneros, University of North Texas, USA
S Coriani, Technical University of Denmark, Denmark
M DeVries, University of California Santa Barbara, USA
C Diaz, Universidad Complutense de Madrid, Spain
J Dupont, University of Nottingham, UK
S Faraji, University of Groningen, Netherlands
D Frenkel, University of Cambridge, UK
A Fujii, Tohoku University, Japan
S George, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), India
R B Gerber, Hebrew University Jerusalem, Israel
D Ghosh, Indian Association for the Cultivation of Science, India
D Goldfarb, Weizmann Institute of Science, Israel
S Grimme, University of Bonn, Germany
M Havenith, Ruhr-University Bochum, Germany
K Holmberg, Chalmers University of Technology, Sweden
Y Iwasawa, University of Tokyo, Japan
D Jacquemin, Université de Nantes, France
T Jagau, KU Leuven, Belgium
E Johnson, Dalhousie University, Canada
J MacPherson, University of Warwick, UK
S.Matsika, Temple University, USA
H Mattoussi, Florida State University, USA
G Meijer, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany
F Neese, Max Planck Institute for Chemical Energy Conversion, Germany
D Nesbitt, University of Colorado, USA
D Neumark, University of California, Berkeley, USA
M Orozco, IRB Barcelona - Parc Científic de Barcelona, Spain
K Pas, Monash University, Australia
G Patwari, Indian Institute of Technology Bombay, India
M-P Pileni, Université Pierre et Marie Curie, France
M Pumera, Nanyang Technological University, Singapore
P Pyykkö, University of Helsinki, Finland
M Rodgers, Wayne State University, USA
S Sampath, Indian Institute of Science Bangalore, India
R Signorell, ETH Zurich, Switzerland
T Schmidt, University of New South Wales, Australia
M Suhm, University of Göttingen, Germany
A Suits, University of Missouri, USA
D Sundholm, University of Helsinki, Finland
T Suzuki, Kyoto University, Japan
A Troisi, University of Warwick, UK
S Vega, Weizmann Institute of Science, Israel
D Waldeck, University of Pittsburgh, USA
L-J Wan, Institute of Chemistry, Chinese Academy of Sciences, China
B Weckhuysen, Utrecht University, The Netherlands
X Yang, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China
A Zehnacker-Rentien, Université Paris, France

Information for Authors

Full details on how to submit material for publication in PCCP are given in the Instructions for Authors (available from **http://www.rsc.org/authors**). Submissions should be made via the journal's **homepage: rsc.li/pccp**

Authors may reproduce/republish portions of their published contribution without seeking permission from the Royal Society of Chemistry, provided that any such republication is accompanied by an acknowledgement in the form: (Original Citation)–Reproduced by permission of the Royal Society of Chemistry.

This journal is © the Owner Societies.
Apart from fair dealing for the purposes of research or private study for non-commercial purposes, or criticism or review, as permitted under the Copyright, Designs and Patents Act 1988 and the Copyright and Related Rights Regulation 2003, this publication may only be reproduced, stored or transmitted, in any form or by any means, with the prior permission in writing of the Publishers or in the case of reprographic reproduction in accordance with the terms of licences issued by the Copyright Licensing Agency in the UK. US copyright law is applicable to users in the USA.

♾ The paper used in this publication meets the requirements of ANSI/NISO Z39.48–1992 (Permanence of Paper).

Registered charity number: 207890

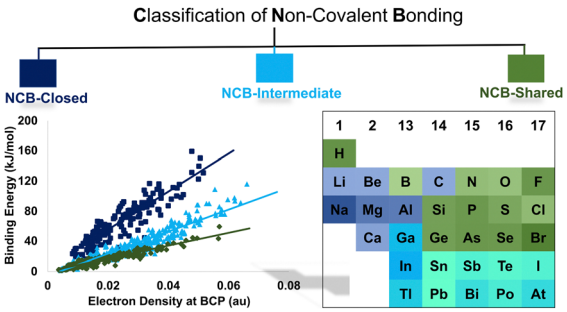
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

PERSPECTIVES

22583

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

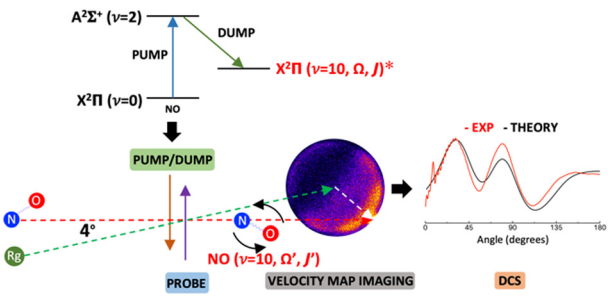
Arijit Das and Elangannan Arunan*



22595

Cold collisions of hot molecules

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

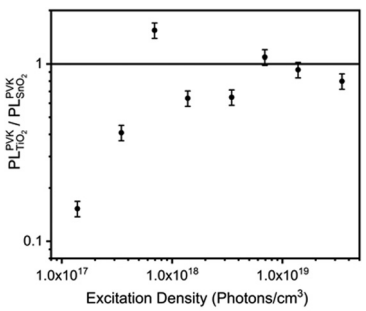


COMMUNICATIONS

22607

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

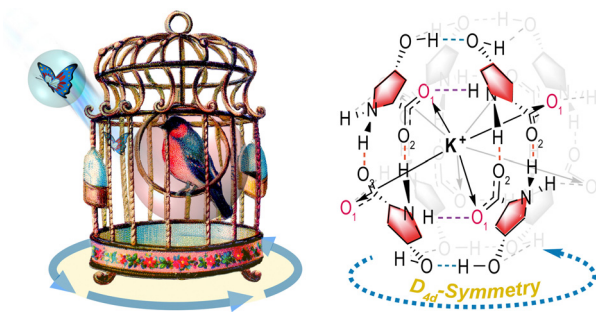
Xinjian Geng, Yawen Liu, Xianshao Zou, Erik M. J. Johansson and Jacinto Sá*



22614

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

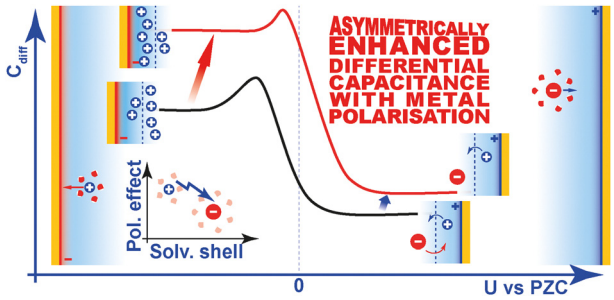
Yameng Hou, Sijin Zhou, Xingshi Xu, Min Kou and Xianglei Kong*



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

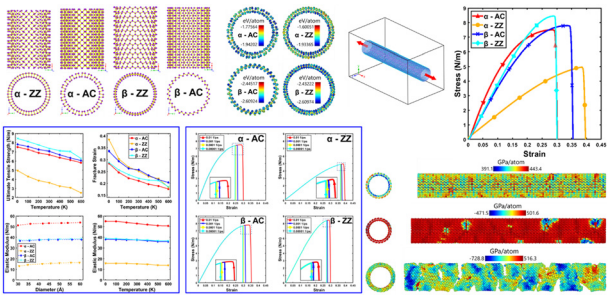
22619



Molecular dynamics simulations of electrified interfaces including the metal polarisation

Samuel Ntim and Marialore Sulpizi*

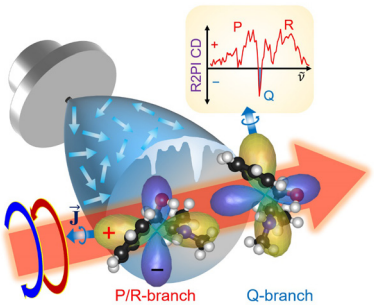
22626



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

Murat Cetin and Mesut Kirca*

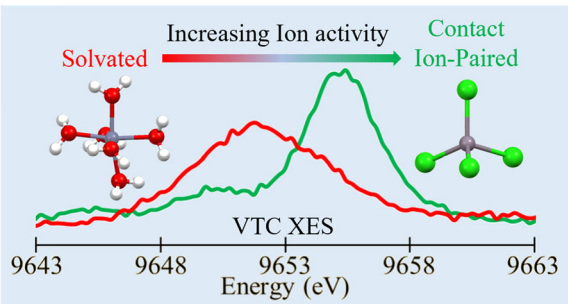
22644



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, Niranjan Govind, Andrew G. Stack, Nikhil Rampal, Gregory Schenter, Christopher J. Mundy, Timothy T. Fister, John L. Fulton, Mahalingam Balasubramanian and Gerald T. Seidler*

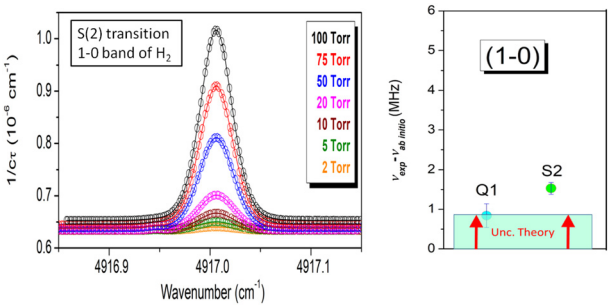
This journal is © the Owner Societies 2023

Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

22662

Accurate absolute frequency measurement of the S(2) transition in the fundamental band of H_2 near 2.03 μm

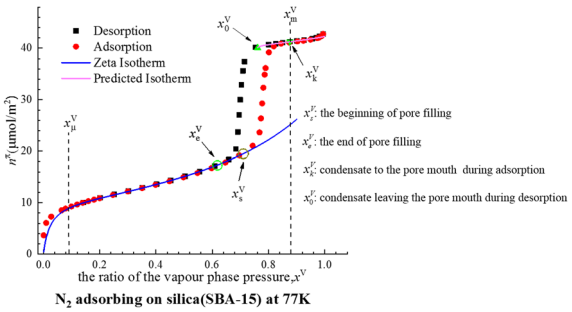
D. Mondelain,* L. Boux de Casson, H. Fleurbaey, S. Kassi and A. Campargue



22669

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

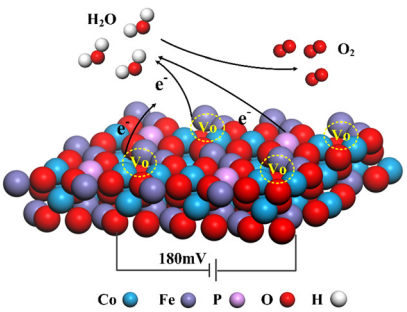
Wei Zhang, Chun-Mei Wu* and You-Rong Li



22679

Cold plasma synthesis of phosphorus-doped $CoFe_2O_4$ with oxygen vacancies for enhanced OER activity

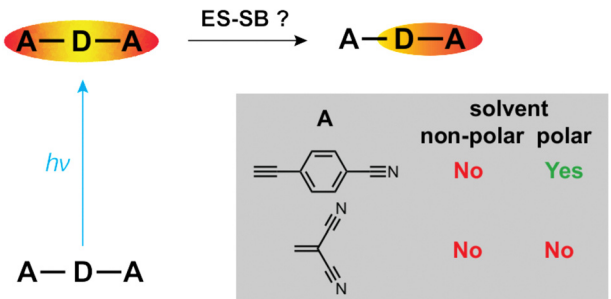
Dapeng Meng, Xiangfeng Peng, Jingxuan Zheng and Zhao Wang*



22689

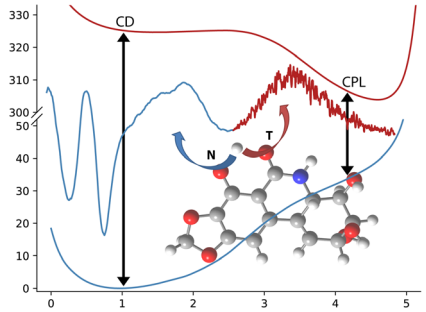
Excited-state symmetry breaking in quadrupolar pull–push–pull molecules: dicyanovinyl *vs.* cyanophenyl acceptors

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



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

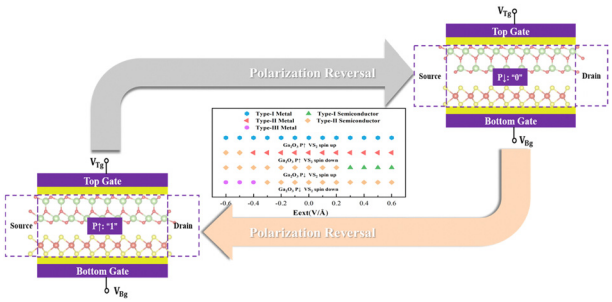
22700



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*

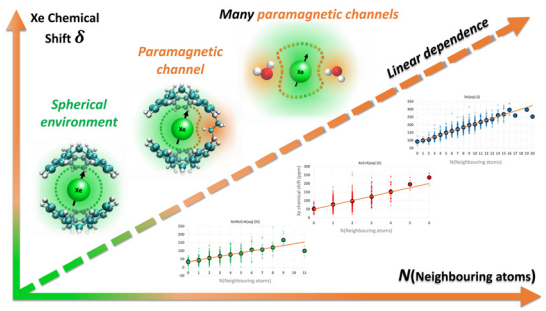
22711



Electrostatic gating dependent multiple band alignments in ferroelectric VS_2/Ga_2O_3 van der Waals heterostructures

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

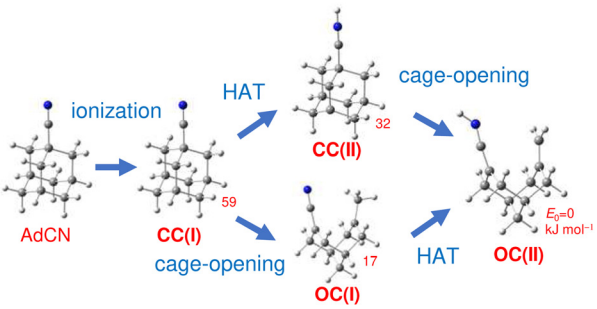
22719



NMR chemical shift of confined ^{129}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*

This journal is © the Owner Societies 2023

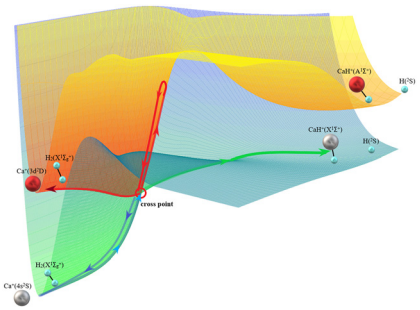
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

22744

The impact of non-adiabatic effects on reaction dynamics: a study based on the adiabatic and non-adiabatic potential energy surfaces of CaH_2^+

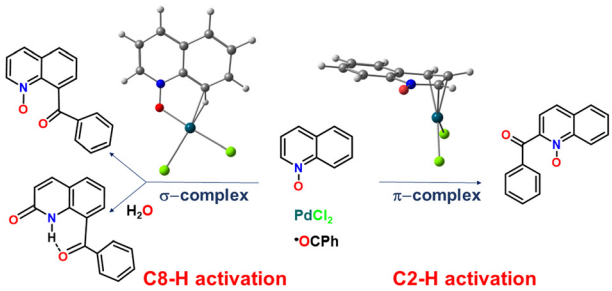
Di He,* Wentao Li, Quanjiang Li, Shenghui Chen, Li Wang, Yanli Liu and Meishan Wang*



22755

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

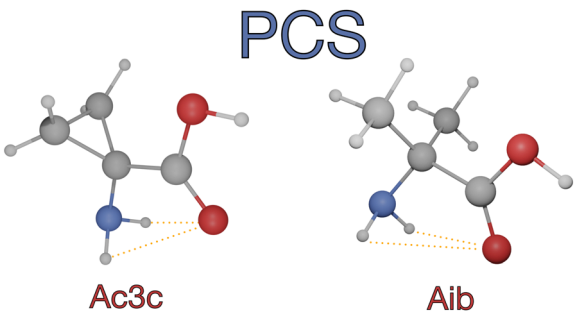
Paulo J. Costa, Frederico F. Martins, Chao Pi, Xiuling Cui and Maria José Calhorda*



22768

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

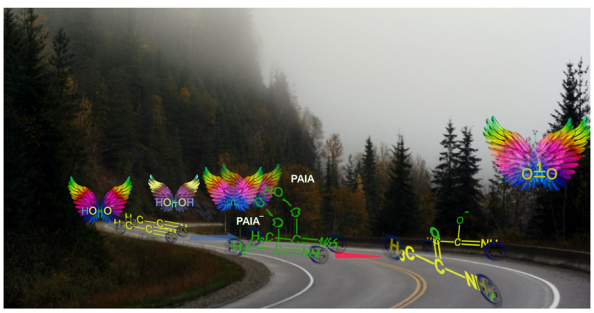
Vincenzo Barone*



22775

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

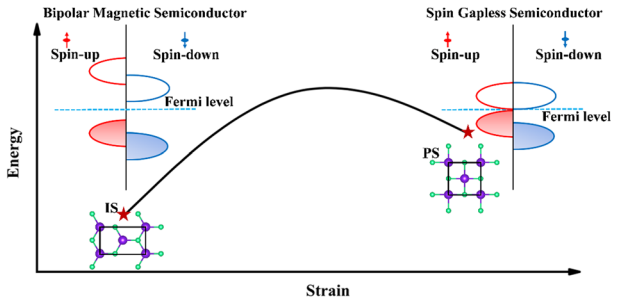
Girolamo Casella,* Silvia Carlotto, Ana P.C. Ribeiro and Luísa M.D.R.S. Martins



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

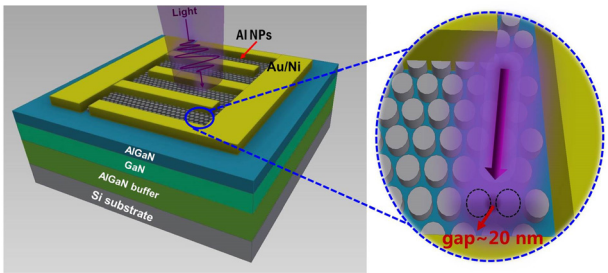
22782



Tunable electrical properties and multiple-phases of ferromagnetic GdS_2, $GdSe_2$ and Janus GdSSe monolayers

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

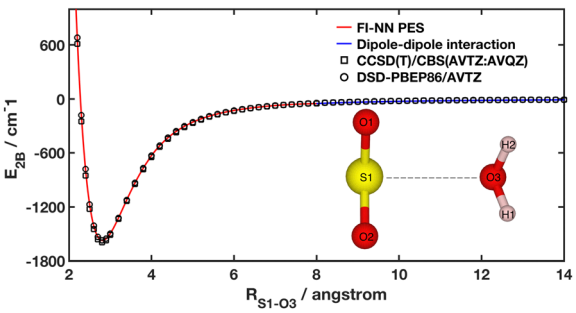
22794



Broadband ultraviolet plasmonic enhanced AlGaN/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*

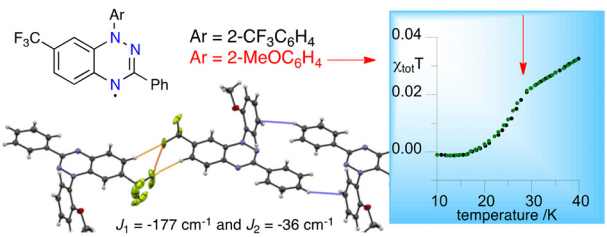
22804



Neural network potential energy surfaces and dipole moment surfaces for $SO_2(H_2O)$ and $SO_2(H_2O)_2$ 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*

This journal is © the Owner Societies 2023

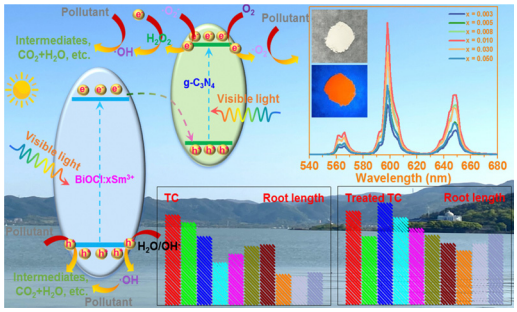
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

22819

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

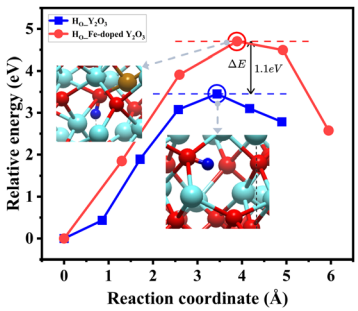
Qian Wu, Xiaoqing Lai, Xiao-Hui Ji, Hai Jiang* and Peng Du*



22832

Trapping and diffusion of hydrogen in iron-doped Y_2O_3

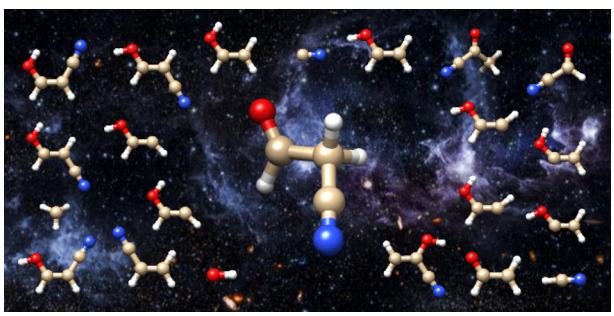
Zhenjie Liu, Zhe Feng, Chunsheng Guo,* Yuxiang Ni, Hongyan Wang, Yuhong Xu and Changjian Tang



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

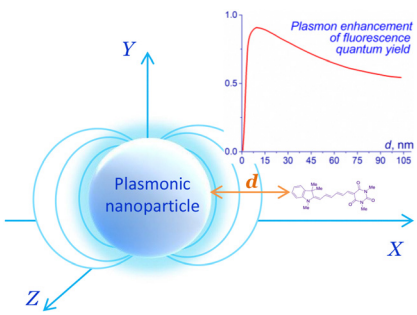
Bernardo Ballotta,* Emilio Martínez-Núñez, Sergio Rampino and Vincenzo Barone*



22851

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

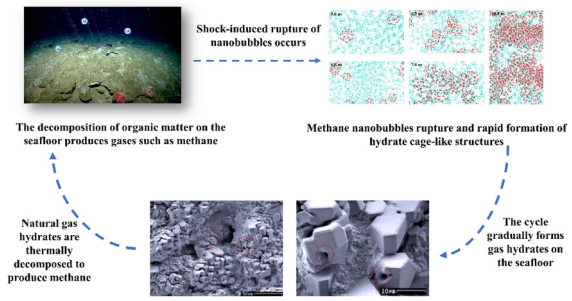
Niyazbek Kh. Ibrayev,* Evgeniya V. Seliverstova, Rashid R. Valiev,* Assel E. Kanapina, Alexander A. Ishchenko, Andrii V. Kulinich, Theo Kurten and Dage Sundholm



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

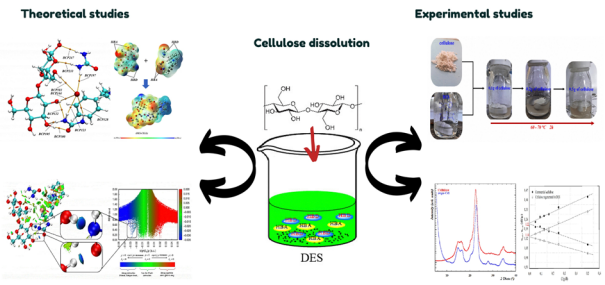
22862



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*

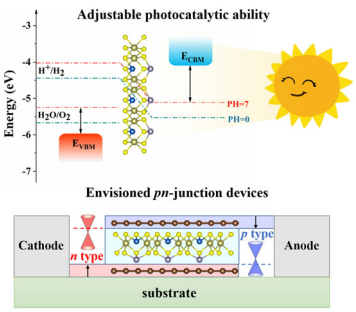
22870



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 Barkany*

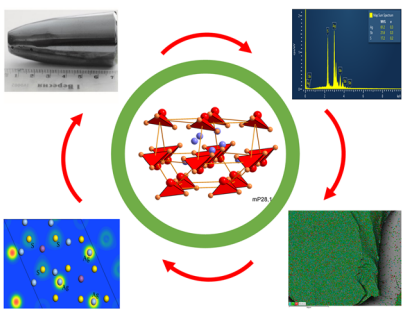
22889



Symmetry-breaking-induced ferroelectric $HfSnX_3$ 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_3SbS_3 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

This journal is © the Owner Societies 2023

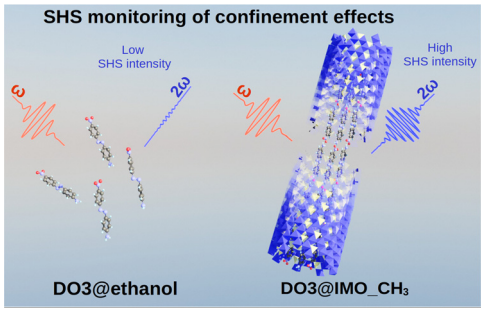
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

22913

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

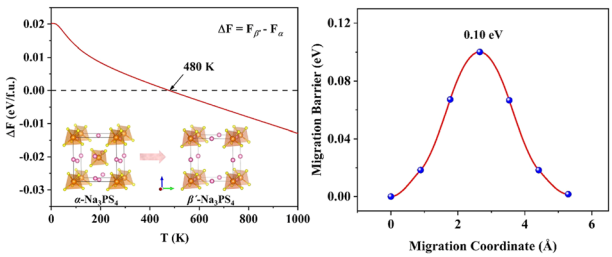
Ali Dhaini, Fadwa Alfadel Raad, Antoine Thill, Benedicte Prelot, Gaelle Martin-Gassin and Pierre-Marie Gassin*



22920

A novel phase of superionic conductor β'-Na_3PS_4 with a large band gap and a low migration barrier

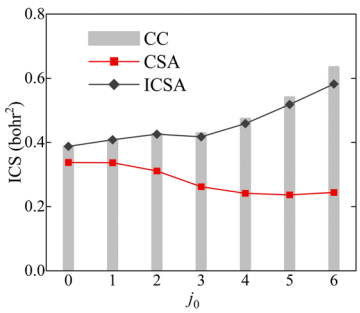
Xiaofeng Zhang, Luo Yan, Qiaoqiao Li, Yongqi Zhang* and Liujiang Zhou*



22927

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

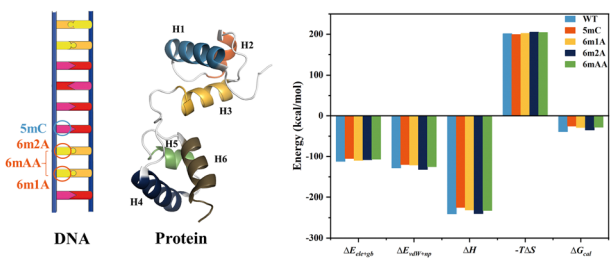
Hanghang Chen, Bayaer Buren, Zijiang Yang and Maodu Chen*



22941

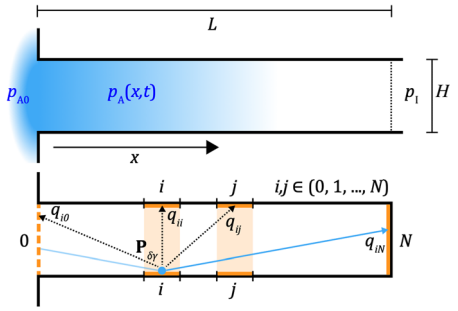
Comprehensive analysis unveils altered binding kinetics of 5-/6-methylCytosine/adenine modifications in R2R3-DNA system

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



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

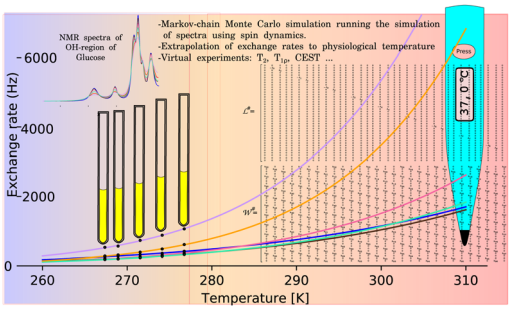
22952



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

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

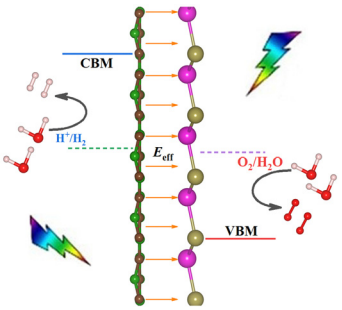
22965



Glucose exchange parameters in a subset of physiological conditions

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

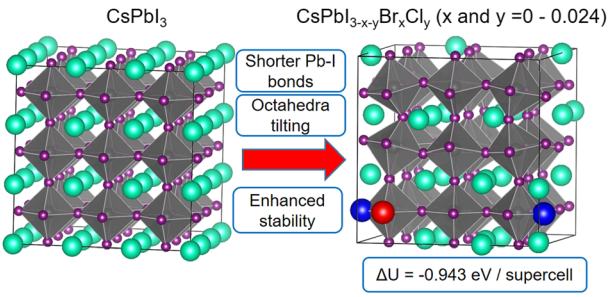
22979



The polarized electric field of $CdTe/B_4C_3$ 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 $CsPbI_{3-x-y}Br_xCl_y$ (x and y = 0–0.024): understanding the role of Cl doping from *ab initio* calculations

Anu Bala* and Vijay Kumar

This journal is © the Owner Societies 2023

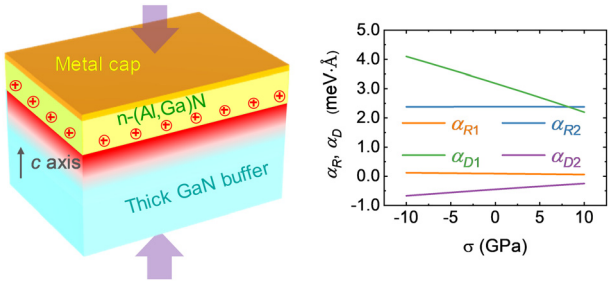
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

23001

Piezoelectric manipulation of spin–orbit coupling in a Wurtzite heterostructure

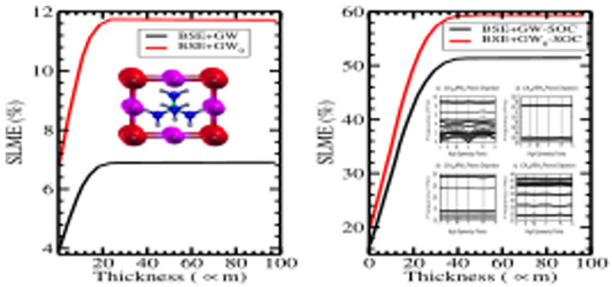
Gongwei Hu,* Fobao Huang and Jun-Feng Liu*



23012

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

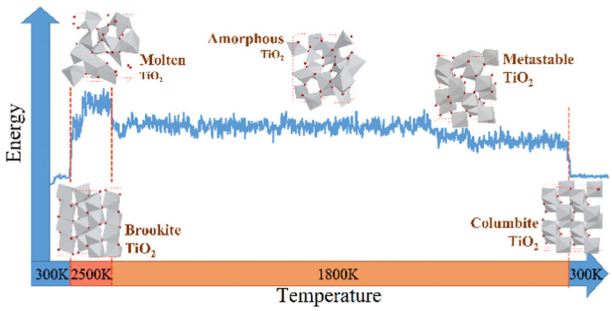
Ridwan O. Agbaoye,* Paul O. Adebambo, Stephane Kenmoe and Gboyega A. Adebayo*



23024

Phase transition of titanium dioxide based on quantum dynamics

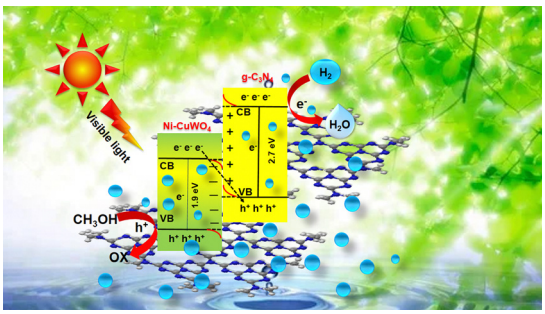
Bing Zhang, Shengbin Chen, Yang Yang, Rui Luo, Yuangu Xia, Xiaogang Wang, Qiang Lu and Bin Hu*



23033

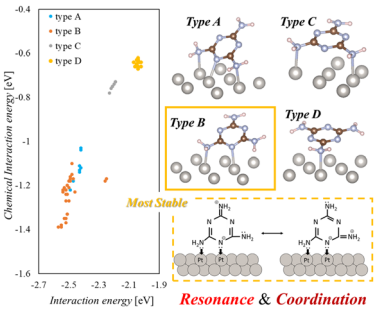
Controlled Ni doping on a g-C_3N_4/$CuWO_4$ photocatalyst for improved hydrogen evolution

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



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

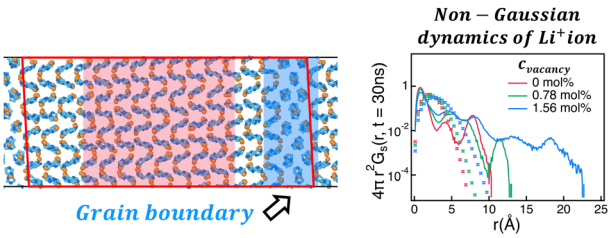
23047



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

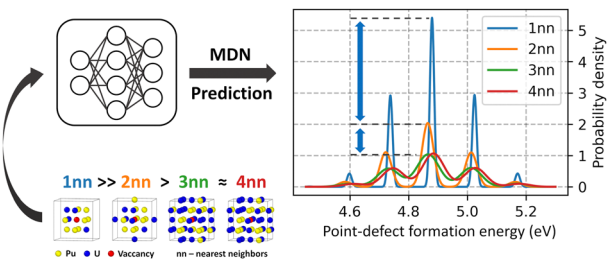
23058



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*

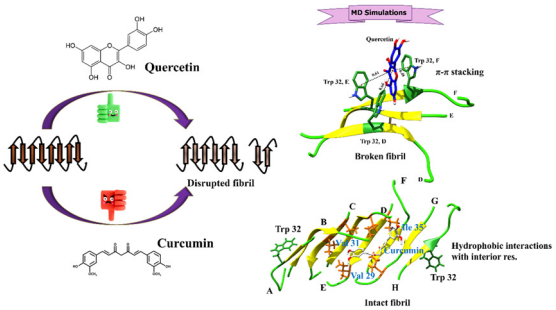
23069



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*

This journal is © the Owner Societies 2023

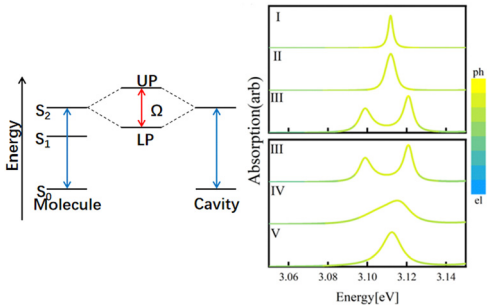
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

23092

Light-responsive organic polaritons from first principles

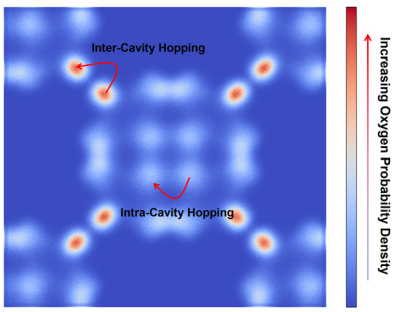
Xiongwei Guo, Xinlu Cheng* and Hong Zhang



23100

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

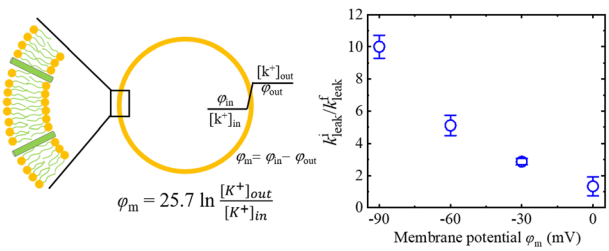
Jing Wang and Shi-Jie Xie*



23111

Increase in anionic Fe_3O_4 nanoparticle-induced membrane poration and vesicle deformation due to membrane potential – an experimental study

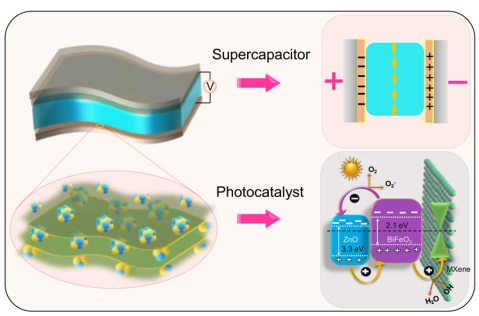
Md. Moniruzzaman, Mohammad Abu Sayem Karal,* Md. Abdul Wadud and Md. Mamun Or Rashid



23125

A MXene–$BiFeO_3$–ZnO nanocomposite photocatalyst served as a high-performance supercapacitor electrode

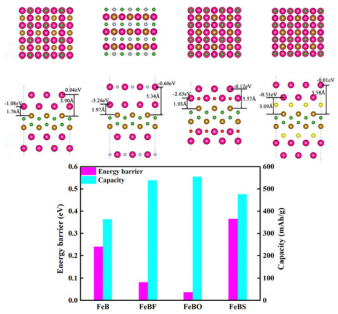
Riya Nag, Sayan Das, Debu Das, Adyam Venimadhav and Abhijit Bera*



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

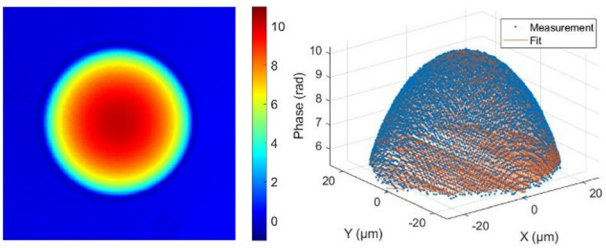
23133



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*

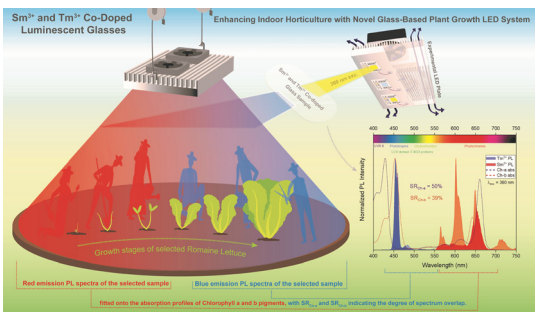
23141



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

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

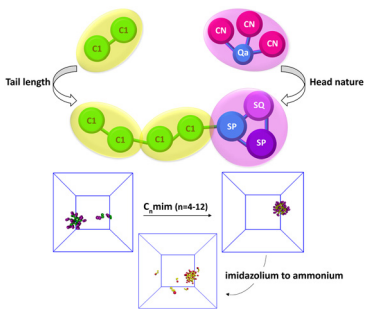
23150



Glass-based LED system for indoor horticulture: enhanced plant growth through Sm^{3+} and Tm^{3+} co-doped luminescent glasses

Utku Ekim, Emre İlter, Emirhan Özan, Yusuf Temürhan, Miray Çelikbilek 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

This journal is © the Owner Societies 2023

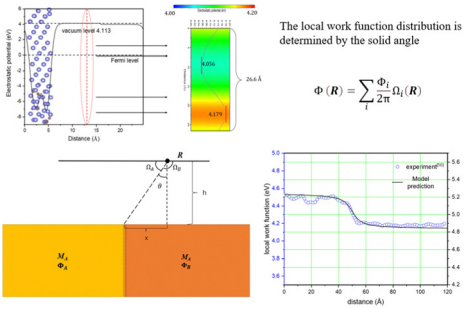
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

23177

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

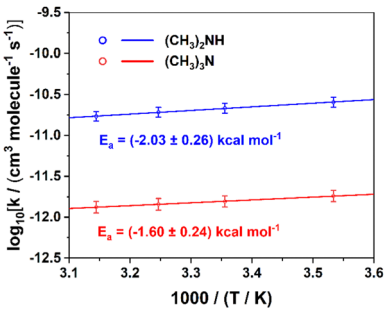
Wenjie Zhou, Chaofang Dong,* Dihao Chen, Li Wang, Xuequn Cheng and Xiaogang Li



23187

The simplest Criegee intermediate CH_2OO reaction with dimethylamine and trimethylamine: kinetics and atmospheric implications

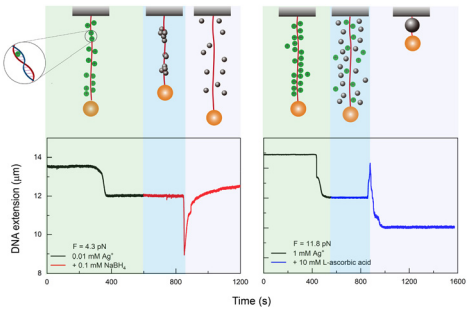
Yang Chen, Licheng Zhong, Siyue Liu, Haotian Jiang, Jiayu Shi, Yuqi Jin, Xueming Yang and Wenrui Dong*



23197

Reductant-dependent DNA-templated silver nanoparticle formation kinetics

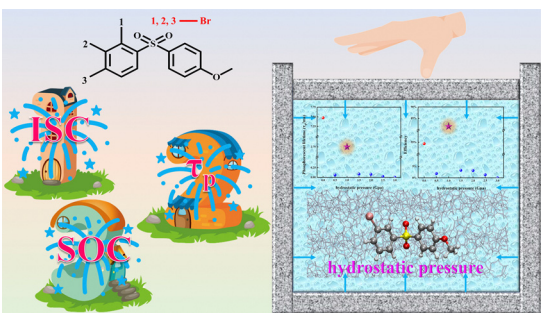
Zi-Yang Yang, Wen-Yan Jiang and Shi-Yong Ran*



23207

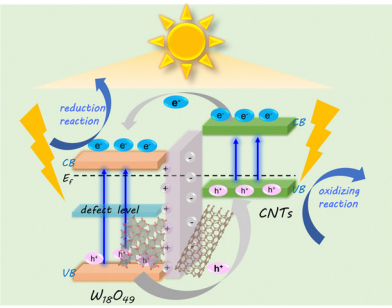
Theoretical exploration of the bromine substitution effect and hydrostatic pressure responsive mechanism for room temperature phosphorescence

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



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

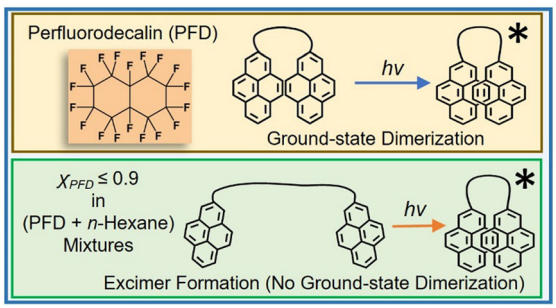
23222



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*

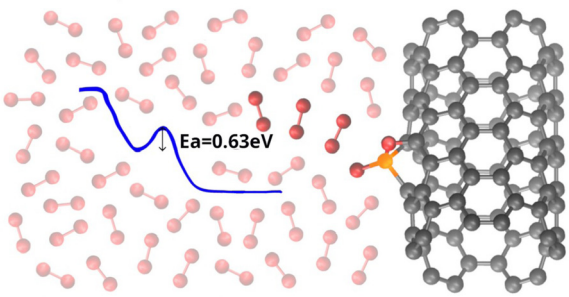
23233



Intramolecular dimer formation reveals anomalous solvation within fluorous solvent perfluorodecalin

Deepika and Siddharth Pandey*

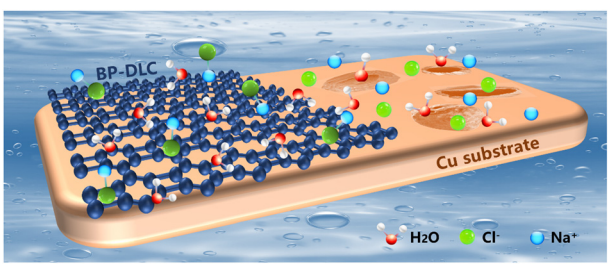
23242



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. Quaino*

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

This journal is © the Owner Societies 2023

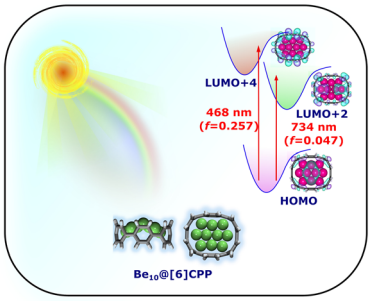
Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

23262

Electronic and photophysical properties of an atomically thin bowl-shaped beryllene encapsulated inside the cavity of [6]cycloparaphenylene (Be_n@[6]CPP)

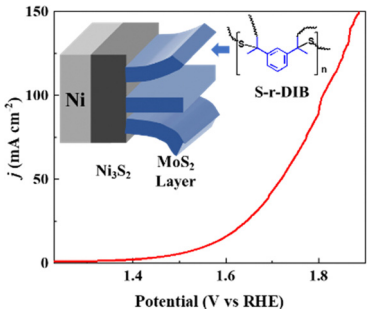
Akanksha Ashok Sangolkar, Rama Krishna Kadiyam, Mohmmad Faizan, Omshireesh Chedupaka, Raghasudha Mucherla and Ravinder Pawar*



23277

Polysulfide induced synthesis of a MoS_2 self-supporting electrode with wide-layer-spacing for efficient electrocatalytic water splitting

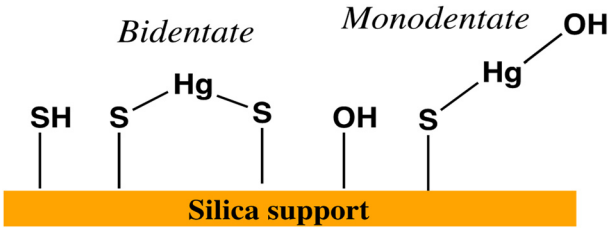
Ningbo Yu, Jianzhi Wang, Hongliang Yu, Daichunzi Yang, Wentao Luo, Xiao Lin, Yanping Liu, Ning Cai, Yanan Xue and Faquan Yu*



23286

Rational design of selective functionalized silica adsorbents for Hg(II) removal from FGD wastewater. A combined experimental and theoretical study

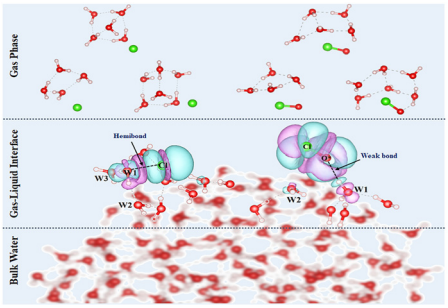
Alma Malibekova and Vadim Guliants*



23296

The effects of the gas–liquid interface and gas phase on Cl/ClO radical interaction with water molecules

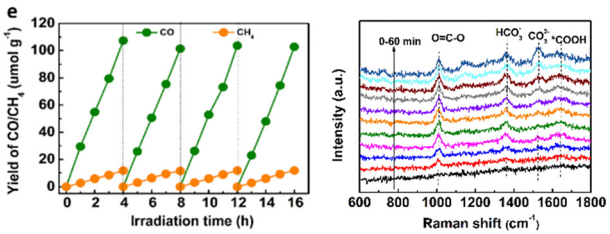
Qi Zhang, Mohammad Hassan Hadizadeh, Yongxia Hu, Xiaoyu Zhang, Zupeng Su, Zihan Wu, Xiaotong Wang, Fei Xu,* Yanhui Sun, Qingzhu Zhang and Wenxing Wang



Open Access Article. Published on 30 August 2023. Downloaded on 7/25/2025 11:48:50 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

RESEARCH PAPERS

23306



Cu-doped mesoporous SnO_2 nanoparticles with rich grain boundaries and oxygen vacancies for photocatalytic CO_2-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*

This journal is © the Owner Societies 2023