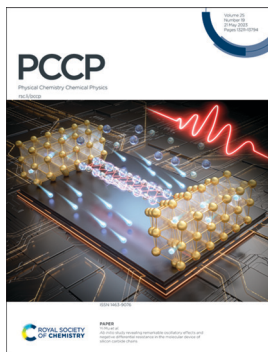


IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(19) 13211–13794 (2023)



Cover

See Yi Mu *et al.*,
pp. 13265–13274.
Image reproduced
by permission of
Yi Mu from
Phys. Chem. Chem. Phys.,
2023, 25, 13265.



Inside cover

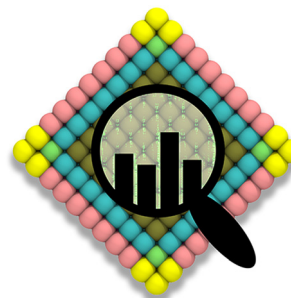
See Sunil Saxena *et al.*,
pp. 13275–13288.
Image reproduced
by permission of
Sunil Saxena from
Phys. Chem. Chem. Phys.,
2023, 25, 13275.

TUTORIAL REVIEW

13228

In silico characterization of nanoparticles

Björn Kirchoff,* Christoph Jung, Daniel Gaissmaier,
Laura Braunwarth, Donato Fantauzzi and Timo Jacob*

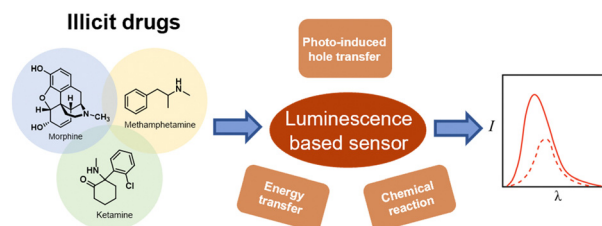


PERSPECTIVE

13244

Luminescence-based detection and identification of illicit drugs

M. Chen, P. L. Burn* and P. E. Shaw*



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, 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 ISSN 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

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-Hoinghaus, 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
I 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

J Janek, Justus Liebig University Giessen, Germany
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 III, University of Georgia, USA (Deputy Chair)
I Tamblin, 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 Neumaier, 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 Pumerla, 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 Weckhuyzen, 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

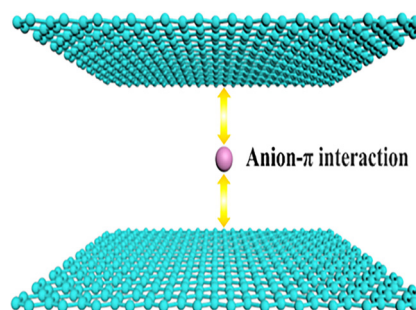


COMMUNICATION

13260

An anomalous anion transfer order in graphene oxide membranes induced by anion- π interactions

Junjie Chen, Jie Li, Xing Liu, Zhenglin He and Guosheng Shi*

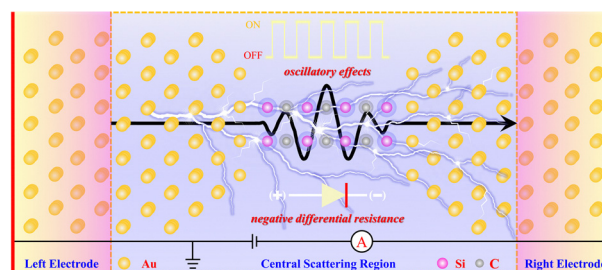


RESEARCH PAPERS

13265

Ab initio study revealing remarkable oscillatory effects and negative differential resistance in the molecular device of silicon carbide chains

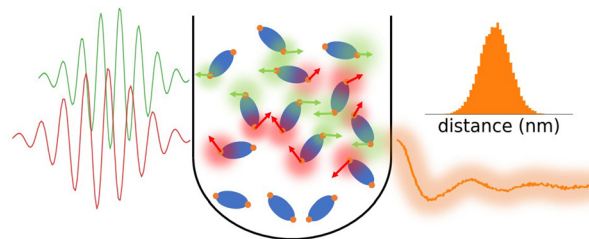
Yi Mu,* Jie Yu, Rui Hu, Cui-Hong Wang, Cai Cheng and Bang-Pin Hou



13275

Efficient sampling of molecular orientations for Cu(II)-based DEER on protein labels

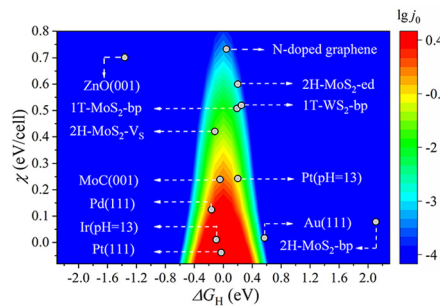
Zikri Hasanbasri, Nicholas A. Moriglioni and Sunil Saxena*



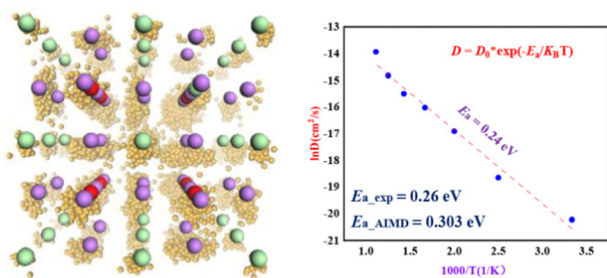
13289

Electronegativity principle for hydrogen evolution activity using first-principles calculations

Yi An, Min Ouyang, Shaoyu Kong, Guangjin Wang and Xiaobo Chen*



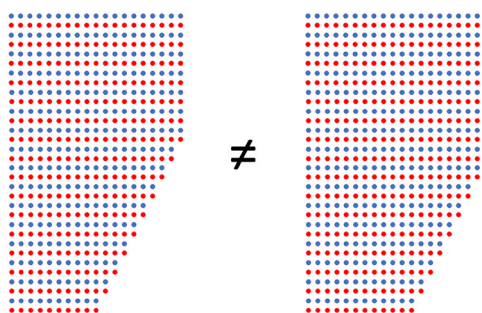
13297



Li ion diffusion behavior of Li_3OCl solid-state electrolytes with different defect structures: insights from the deep potential model

Zhou Zhang, Zhongyun Ma* and Yong Pei*

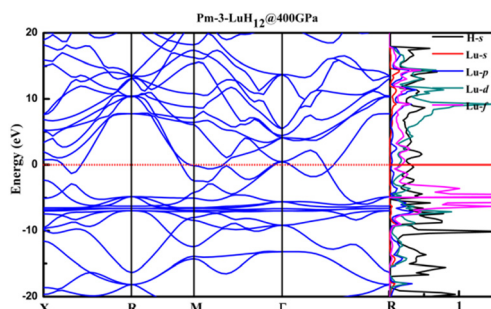
13308



The shape effect and its consequences for polar surfaces and for heterogeneous catalysis

Michael Springborg,* Meijuan Zhou and Bernard Kirtman

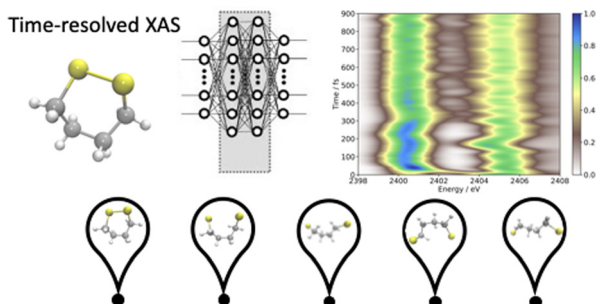
13320



Pressure-induced stability and superconductivity in LuH_{12} polyhydrides

Junyi Du, Weiguo Sun, Xiaofeng Li and Feng Peng*

13325

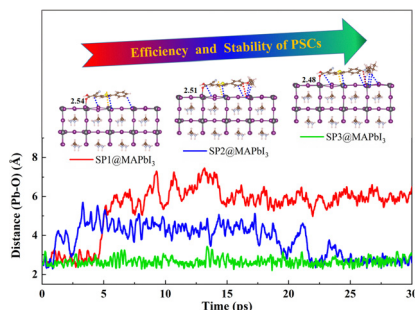


An on-the-fly deep neural network for simulating time-resolved spectroscopy: predicting the ultrafast ring opening dynamics of 1,2-dithiane

Clelia Middleton, Conor D. Rankine and Thomas J. Penfold*



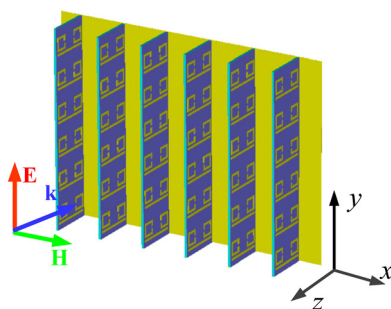
13383



Cooperative multiple interactions of donor- π -acceptor dyes enhance the efficiency and stability of perovskite solar cells

Xiufang Hou,* Weiyi Zhang and Quan-Song Li*

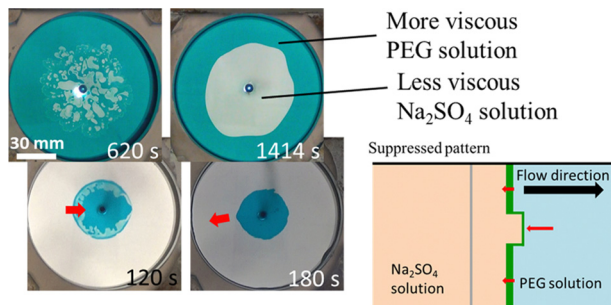
13393



Tunable and three-dimensional dual-band metamaterial absorber based on electromagnetically induced transparency with vanadium dioxide

Mingming Chen* and Xue-Xia Yang*

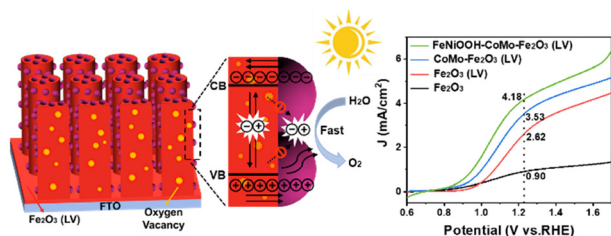
13399



Experimental demonstration of the suppression of viscous fingering in a partially miscible system

Kaori Iwasaki, Yuichiro Nagatsu, Takahiko Ban, Jun Iijima, Manoranjan Mishra and Ryuta X. Suzuki*

13410



CoMoO₄-modified hematite with oxygen vacancies for high-efficiency solar water splitting

Gaoteng Zhang, Cheng Lu, Chang Li, Shuo Li, Xiaoquan Zhao, Kaiqi Nie, Jiaou Wang, Kun Feng* and Jun Zhong*

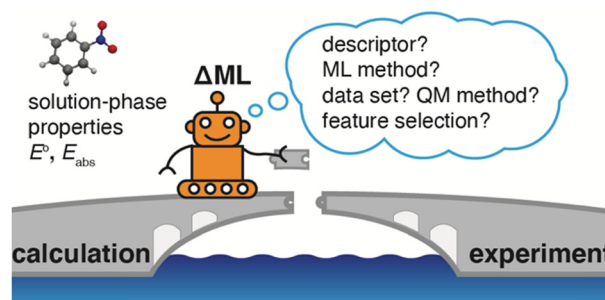


RESEARCH PAPERS

13417

Δ -Machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states

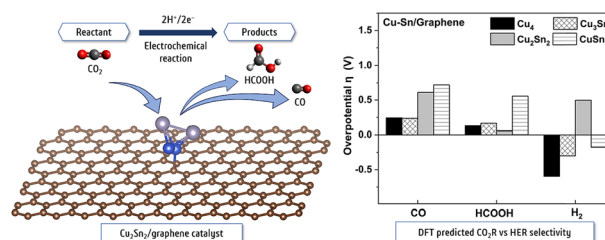
Xu Chen, Pinyuan Li, Eugen Hruska and Fang Liu*



13429

Adsorption, activation, and conversion of carbon dioxide on small copper–tin nanoclusters

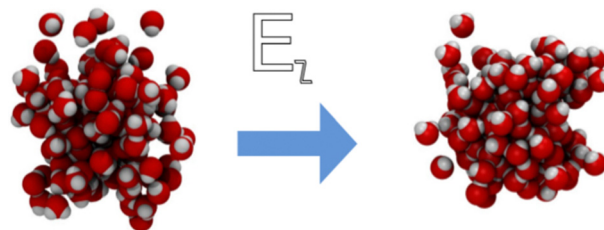
Akshayini Muthuperianayagam, Azeem Ghulam Nabi, Qi Zhao, Aman-ur-Rehman and Devis Di Tommaso*



13442

Vibrational dynamics of liquid water in an external electric field

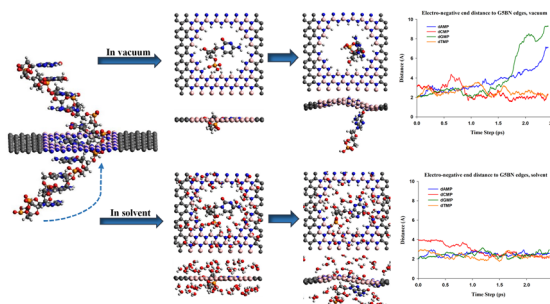
Deepak Ojha* and Thomas D. Kühne



13452

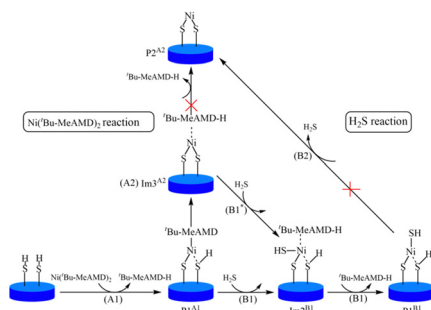
Exploring the dynamics of DNA nucleotides in graphene/h-BN nanopores: insights from *ab initio* molecular dynamics

Ali Kiakojouri, Irmgard Frank and Ebrahim Nadimi*



RESEARCH PAPERS

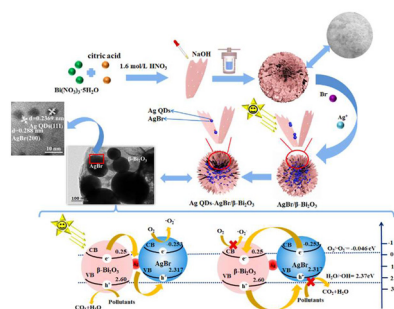
13465



Reaction mechanism of nickel sulfide atomic layer deposition using bis(*N,N'*-di-*tert*-butylacetamidinato)nickel(II) and hydrogen sulfide

Xu Zhang, Zhongchao Zhou, Rui Xu, Jiayi Guo, Lina Xu,*
Yihong Ding, Hongping Xiao, Xinhua Li, Aidong Li and
Guoyong Fang*

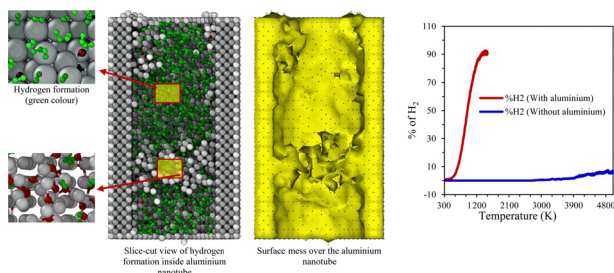
13474



Construction of a Z-scheme heterojunction bifunctional photocatalyst with Ag-modified AgBr embedded in β - Bi_2O_3 flowers

Xin Guan, Xiao-li Wang, Xue-wen Zhu, Hui Yu,*
Ming Yang, Xiang-ting Dong,* Ying Yang* and Long Xia*

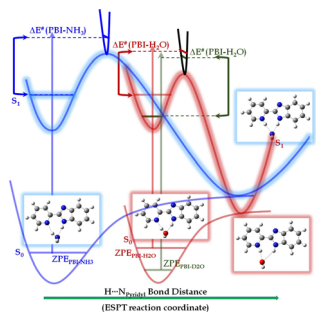
13487



Aluminum nanotubes as an efficient catalyst for hydrogen production via thermochemical water splitting: a reactive molecular dynamics simulation

Sunil Kumar* and Ranjan K. Sahu

13498



Excited-state deactivation via solvent-to-chromophore proton transfer in an isolated 1:1 molecular complex: experimental validation by measuring the energy barrier and kinetic isotope effect

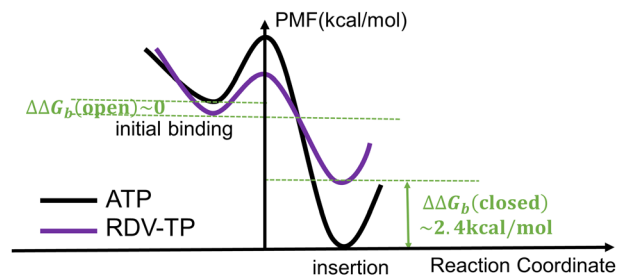
Saurabh Khodia, Ramesh Jarupula, Simran Baweja,
Muhammed Shabeeb, Bhavika Kalal and Surajit Maity*



13508

Energetic vs. entropic stabilization between a Remdesivir analogue and cognate ATP upon binding and insertion into the active site of SARS-CoV-2 RNA dependent RNA polymerase

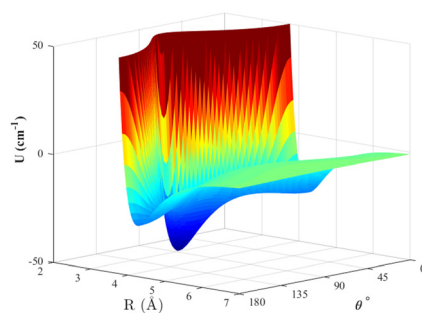
Chunhong Long, Moises Ernesto Romero, Liqiang Dai and Jin Yu*



13521

Quantum mechanical and classical calculation of the transport and relaxation properties of He ··· CO₂ complex using a new PES

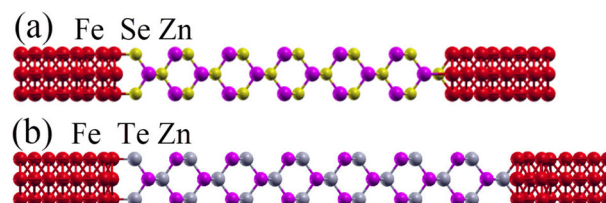
Ebrahim Nemati-Kande,* Fatemeh Aghababaei and Salar Sadeghi



13533

ZnSe and ZnTe as tunnel barriers for Fe-based spin valves

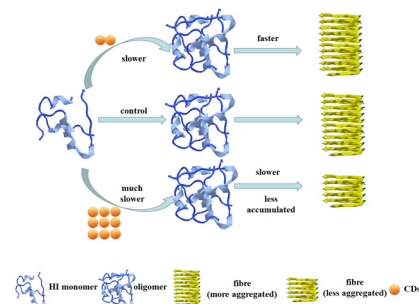
Gokaran Shukla, Hasan M. Abdullah, Avijeet Ray, Shubham Tyagi, Aurélien Manchon, Stefano Sanvito and Udo Schwingenschlögl*



13542

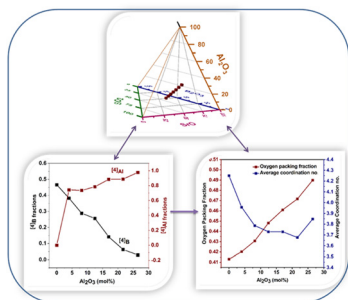
Regulation mechanism of human insulin fibrillation by L-lysine carbon dots: low concentration accelerates but high concentration inhibits the fibrillation process

Xing-Yu Liu, Shuai-Chen Du, Feng-Lei Jiang, Peng Jiang* and Yi Liu*



RESEARCH PAPERS

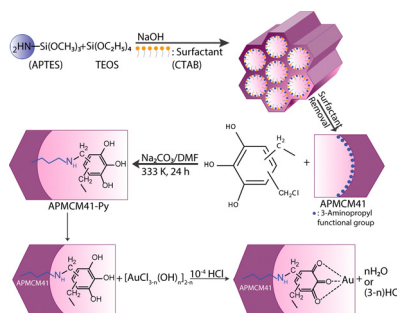
13550



An investigation of Al₂O₃ induced variations in the structural parameters in strontium borosilicate glasses using solid state NMR

Kavya Illath, Prasanta K. Ojha, Sangram K. Rath and T. G. Ajithkumar*

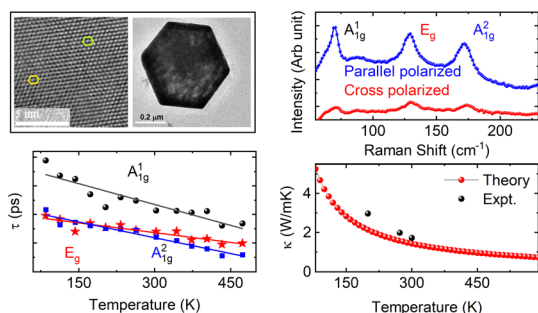
13560



Optimization of Au(III) adsorption by the Taguchi method using pyrogallol functionalized silica nanoparticles

Mustafa Can,* Engin Deniz Parlar, Mustafa Akçil, Abdülkadir Kızıllarlan, Semra Boran, Abdullah Hulusi Kökçam and Özer Uygun

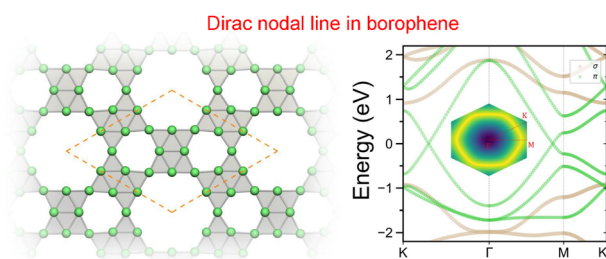
13577



Lattice thermal conductivity of topological insulator Bi₂Se₃ nanocrystals: comparison from theoretical and experimental

Vipin K. E., Soumendra Kumar Das and Prahallad Padhan*

13587



A two-dimensional borophene monolayer with ideal Dirac nodal-line fermions

Chengyong Zhong,* Xuelian Li, Chunbao Feng and Peng Yu*

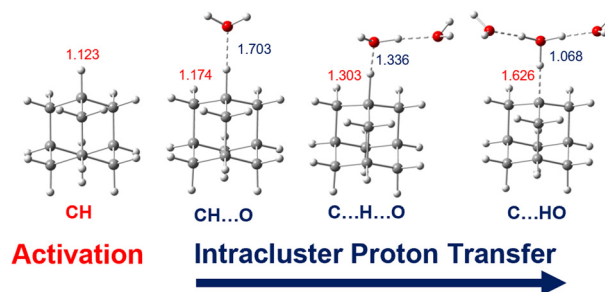


RESEARCH PAPERS

13593

Microhydration of the adamantane cation: intracuster proton transfer to solvent in $[\text{Ad}(\text{H}_2\text{O})_{n=1-5}]^+$ for $n \geq 3$

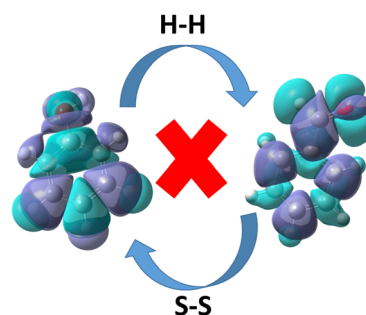
Martin Andreas Robert George and Otto Dopfer*



13611

Can we predict ambident regioselectivity using the chemical hardness?

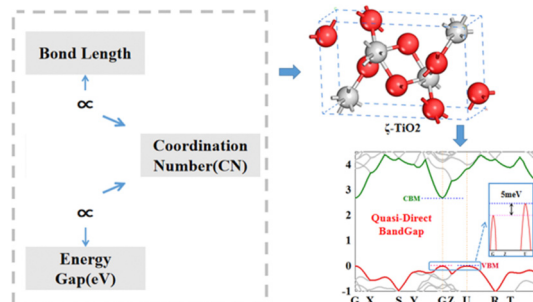
Ramón Alain Miranda-Quintana,* Alberto Vela, Frank De Proft, Marco Martínez González and José L. Gázquez



13623

Novel three-dimensional TiO_2 structure with a unique quasi-direct band gap for photocatalysts

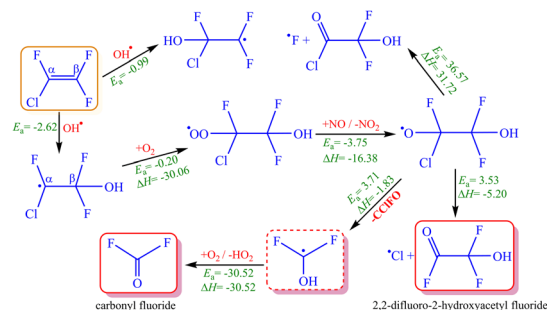
Jiayi Guo, Wangping Xu, Juexian Cao* and Xiaolin Wei*



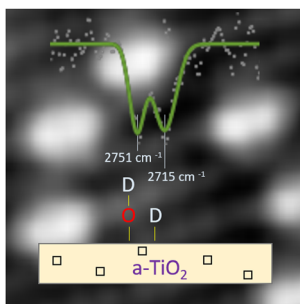
13630

Understanding the kinetics and atmospheric degradation mechanism of chlorotrifluoroethylene ($\text{CF}_2=\text{CFCl}$) initiated by OH radicals

Saber Safari Balsini, Abolfazl Shiroudi,* Farhad Hatamjafari,* Ehsan Zahedi, Khalil Pourshamsian and Ahmad Reza Oliaey



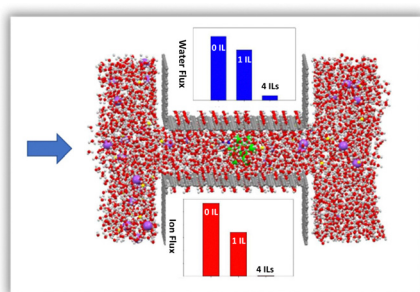
13645



Origin of hydroxyl pair formation on reduced anatase TiO₂(101)

Kræn C. Adamsen, Nikolay G. Petrik,* Wilke Dononelli, Greg A. Kimmel, Tao Xu, Zheshen Li, Lutz Lammich, Bjørk Hammer, Jeppe V. Lauritsen and Stefan Wendt*

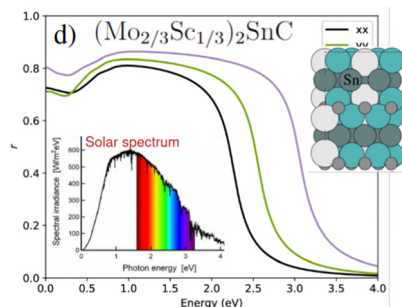
13654



Polyoxometalate ionic liquid between graphene oxide surfaces as a new membrane in the desalination process: a molecular dynamics study

Mohsen Abbaspour

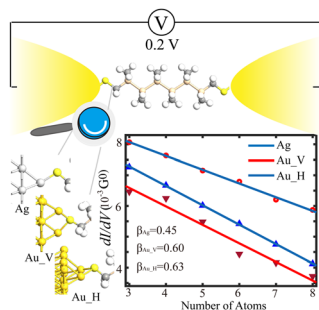
13665



Optical properties of in-plane chemically ordered *i*-MAX structures

Junais Habeeb Mokkath

13673



Silver electrodes provide higher conductance than gold for thiol-terminated oligosilane molecular junctions: the interfacial effect

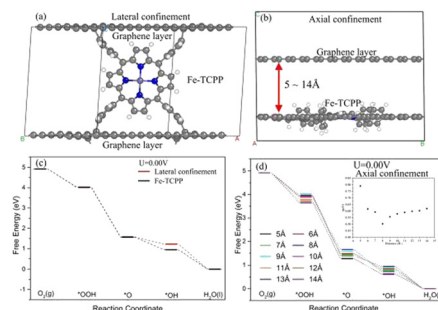
Minglang Wang,* Xianglin Chen, Wenjun Lu, Xinyue Tian and Guang-Ping Zhang



13683

Exploration of spatial confinement and ligand effects for the oxygen reduction reaction on Fe–N_x embedded hole-graphene

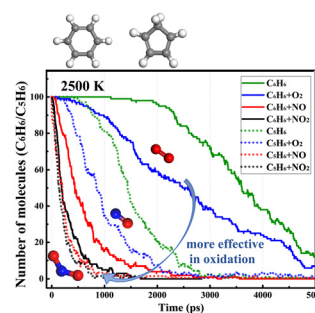
Jing-Hua Guo,* Hong-Bo Wang, Hai-Ying Liu, Gang Chen* and Ting-Ting Cao



13690

Pyrolysis and oxidation of benzene and cyclopentadiene by NO_x: a ReaxFF molecular dynamics study

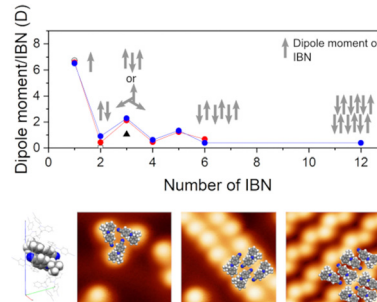
Ying Wang, Lei Zhou, Qian Mao,* Zhanyuan Wang and Haiqiao Wei*



13702

Dipole-moment-induced supramolecular assembly of a donor–acceptor-type molecule on a metal surface and in a crystal

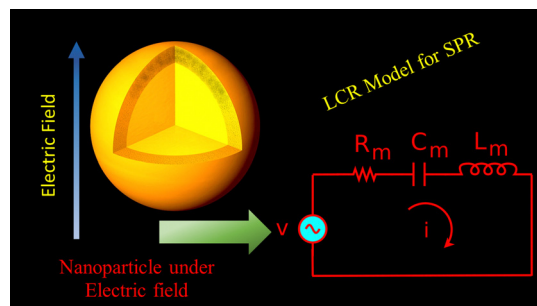
W. Nakanishi,* Y. Matsushita, M. Takeuchi and K. Sagisaka*



13708

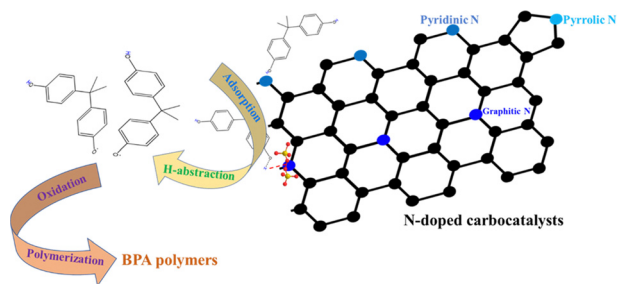
Surface plasmon resonance in metal nanospheres explained with LCR circuits

Shivangi Dubey, Kuldeep Kumar* and P. Arun



RESEARCH PAPERS

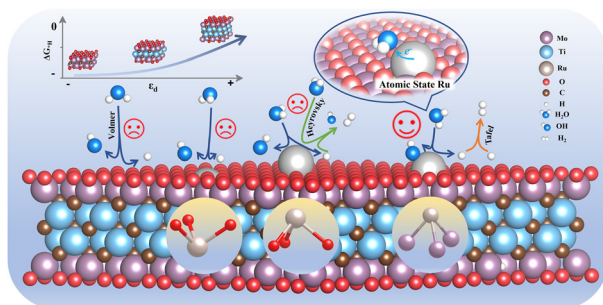
13716



Nitrogen-doped carbocatalyst activated persulfate (PS) for oxidation polymerization of bisphenol A (BPA): importance of nonradical activation of PS

Caihong Wang, Yong Liu,* Fengshen Han, Yongzhe Han, Tianyu Liu, Haitao Ren and Xu Han*

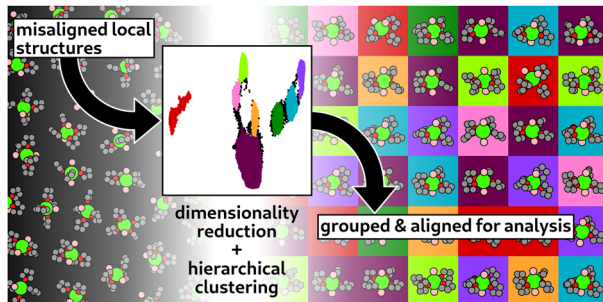
13728



Single atom supported on MXenes for the alkaline hydrogen evolution reaction: species, coordination environment, and action mechanism

Zijun Sun, Rui Li,* Qing Xi, Fangxia Xie, Xuan Jian, Xiaoming Gao, Houfen Li, Zhuobin Yu, Jianxin Liu, Xiaochao Zhang, Yawen Wang, Yunfang Wang, Xiuping Yue* and Caimei Fan

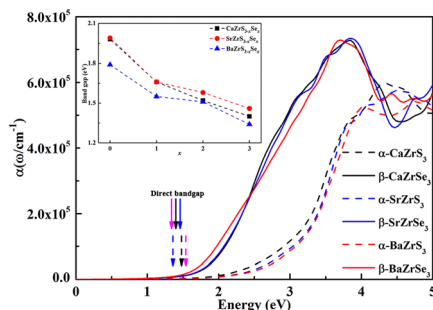
13741



Unsupervised learning of representative local atomic arrangements in molecular dynamics data

Fabrice Roncoroni, Ana Sanz-Matias, Siddharth Sundararaman and David Prendergast*

13755



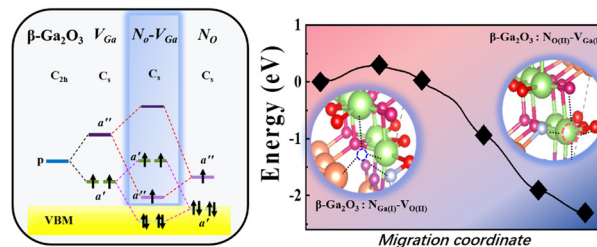
Computational study of the fundamental properties of Zr-based chalcogenide perovskites for optoelectronics

Diwen Liu,* Huihui Zeng, Huan Peng and Rongjian Sa*

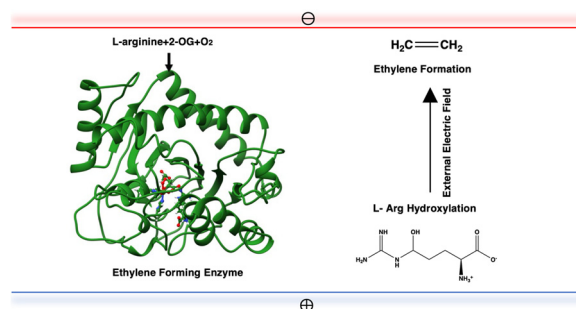


RESEARCH PAPERS

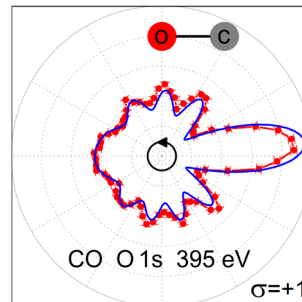
13766

P-type nitrogen-doped β -Ga₂O₃: the role of stable shallow acceptor N_O-V_{Ga} complexesCongcong Ma, Zhengyuan Wu, Hao Zhang,*
Heyuan Zhu, Junyong Kang, Junhao Chu and Zhilai Fang*

13772

Can an external electric field switch between ethylene formation and L-arginine hydroxylation in the ethylene forming enzyme?Shobhit S. Chaturvedi, Simahudeen Bathir
Jaber Sathik Rifayee, Rajeev Ramanan, Joel A. Rankin,
Jian Hu, Robert P. Hausinger and Christo Z. Christov*

13784

High-energy molecular-frame photoelectron angular distributions: a molecular bond-length rulerI. Vela-Peréz, F. Ota, A. Mhamdi, Y. Tamura, J. Rist,
N. Melzer, S. Uerken, G. Nalin, N. Anders, D. You,
M. Kircher, C. Janke, M. Waitz, F. Trinter,* R. Guillemin,
M. N. Piancastelli, M. Simon, V. T. Davis, J. B. Williams,
R. Dörner, K. Hatada, K. Yamazaki, K. Fehre,
Ph. V. Demekhin,* K. Ueda, M. S. Schöffler and T. Jahnke*

CORRECTION

13792

Correction: Crystalline matrix-activated spin-forbidden transitions of engineered organic crystals

Heming Zhang, Lianbao Ke, Yufang Nie, Zhengqian Tu, Jiaxuan Wang, Semion K. Saikin, Hai Bi* and Yue Wang

