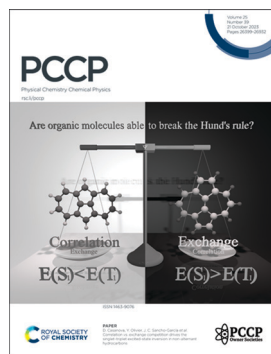


IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 25(39) 26399–26932 (2023)



Cover

See D. Casanova, Y. Olivier, J. C. Sancho-García *et al.*, pp. 26417–26428. Image reproduced by permission of Gaetano Ricci from *Phys. Chem. Chem. Phys.*, 2023, 25, 26417.



Inside cover

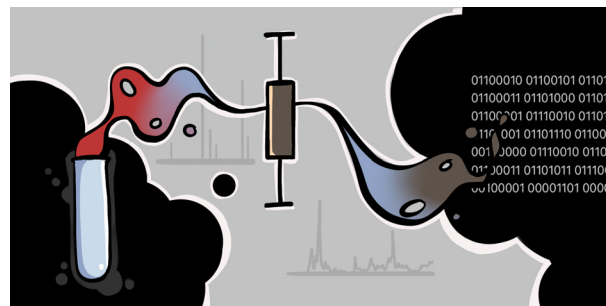
See David de Sancho, Xabier Lopez *et al.*, pp. 26429–26442. Image reproduced by permission of Xabier Lopez and David de Sancho from *Phys. Chem. Chem. Phys.*, 2023, 25, 26429.

EDITORIAL

26415

Benchmark experiments for numerical quantum chemistry

Ricardo A. Mata, Anne Zehnacker-Rentien and Martin A. Suhm

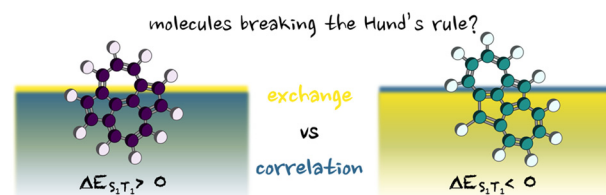


RESEARCH PAPERS

26417

Correlation vs. exchange competition drives the singlet–triplet excited-state inversion in non-alternant hydrocarbons

M. E. Sandoval-Salinas, G. Ricci, A. J. Pérez-Jiménez, D. Casanova,* Y. Olivier* and J. C. Sancho-García*



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 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
L Bañares, Universidad Complutense de Madrid, Spain
M Curri, University of Bari, Italy
C Daniel, Institute of Chemistry, University of Strasbourg, France
L Goerigk, The University of Melbourne, Australia
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
S Matsika, Temple University, USA
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 Neumarck, 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 Pyrykkö, 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 Weckhuesen, 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

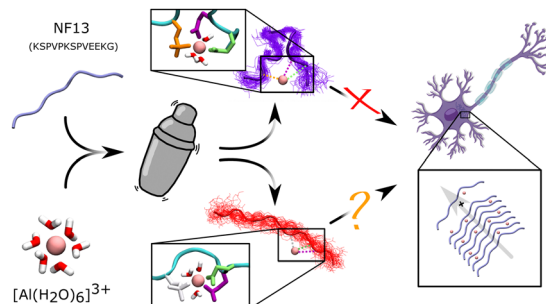


RESEARCH PAPERS

26429

Influence of metal binding on the conformational landscape of neurofilament peptides

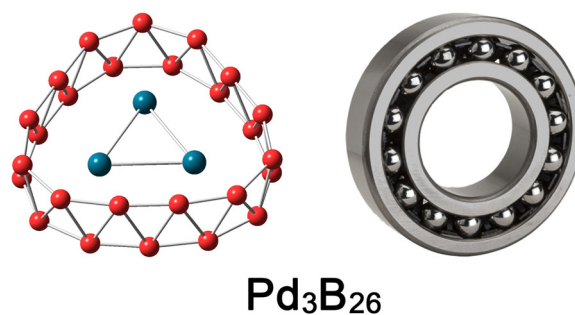
David Silva-Brea, David de Sancho* and Xabier Lopez*



26443

Boron-based Pd₃B₂₆ alloy cluster as a nanoscale antifriction bearing system: tubular core-shell structure, double π/σ aromaticity, and dynamic structural fluxionality

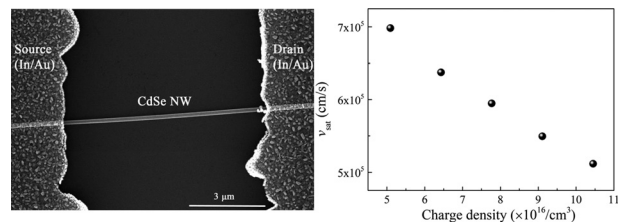
Lin-Yan Feng, Jin-Chang Guo, Ying-Jin Wang, Xiao-Ying Zhang and Hua-Jin Zhai*



26455

Drift velocity saturation in field-effect transistors based on single CdSe nanowires

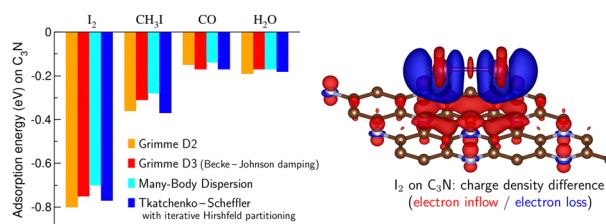
Weifeng Jin* and Xinyang Yang



26461

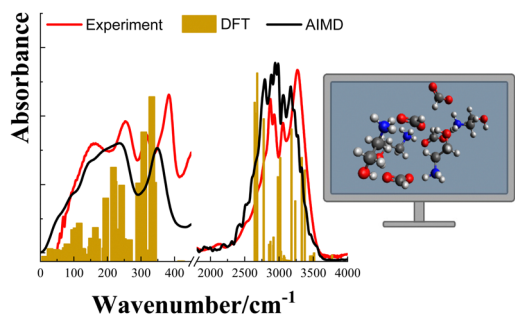
Potential of nanostructured carbon materials for iodine detection in realistic environments revealed by first-principles calculations

Kazem Zhou, Ayoub Daouli, Andrei Postnikov,* Abdellatif Hasnaoui and Michael Badawi*



RESEARCH PAPERS

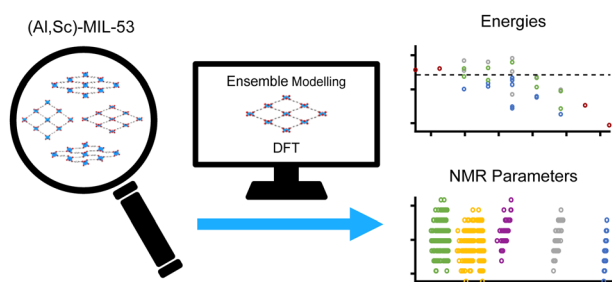
26475



DFT and *ab initio* molecular dynamics simulation study of the infrared spectrum of the protic ionic liquid 2-hydroxyethylammonium formate

Vitor Hugo Paschoal and Mauro C. C. Ribeiro*

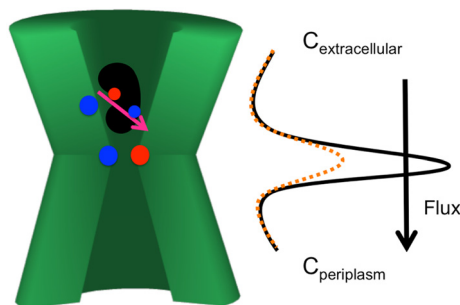
26486



Computational NMR investigation of mixed-metal (Al,Sc)-MIL-53 and its phase transitions

Zachary H. Davis, Emma A. L. Borthwick, Russell E. Morris* and Sharon E. Ashbrook*

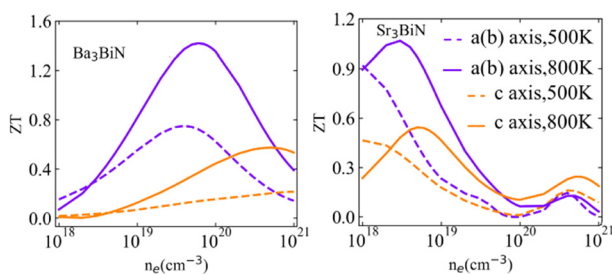
26497



The mechanism of an electrostatic nanofilter: overcoming entropy with electrostatics

Igor Bodrenko, Matteo Ceccarelli* and Silvia Acosta-Gutierrez

26507



Low lattice thermal conductivities and good thermoelectric performance of hexagonal antiperovskites X(Ba & Sr)₃BiN with quartic anharmonicity

Shuming Zeng,* Xiang Yan, Qian Shen, Yusong Tu, Hao Huang* and Geng Li*

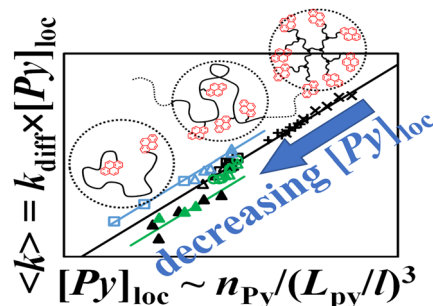


RESEARCH PAPERS

26515

Probing the inner local density of complex macromolecules by pyrene excimer formation

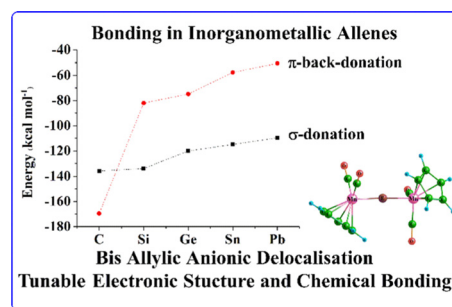
Hunter Little, Sanjay Patel and Jean Duhamel*



26526

Inorganometallic allenes $[(Mn(\eta^5-C_5H_5)(CO)_2)_2(\mu-E)]$ (E = Si–Pb): bis-allylic anionic delocalisation similar to organometallic allene but differential σ -donation and π -backdonation

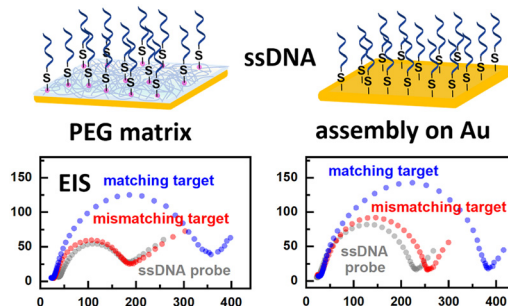
Parameswaran Parvathy and Pattiyil Parameswaran*



26538

Exploiting epoxy-rich poly(ethylene glycol) films for highly selective ssDNA sensing via electrochemical impedance spectroscopy

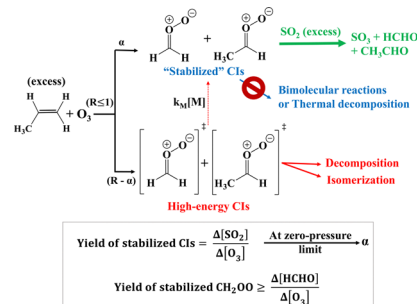
Zhiyong Zhao and Michael Zharnikov*



26549

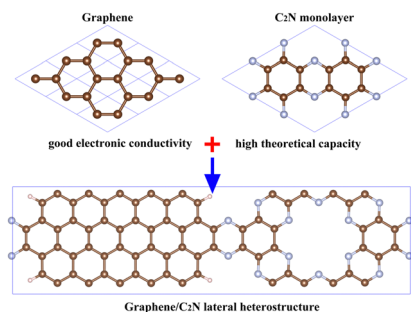
Low-pressure and nascent yields of stabilized Criegee intermediates CH_2OO and CH_3CHOO in ozonolysis of propene

Lei Yang, Mixtli Campos-Pineda, Katia Hatem and Jingsong Zhang*



RESEARCH PAPERS

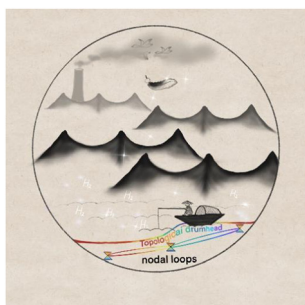
26557



Graphene/C₂N lateral heterostructures as promising anode materials for lithium-ion batteries

Yawen Chen, Qianru Wang, Quan Zhang, Shengli Zhang and Yang Zhang*

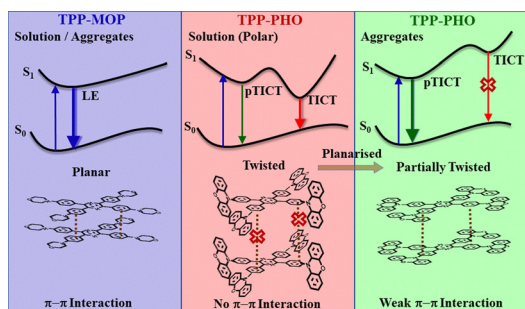
26566



Drumhead surface states promoted hydrogen evolution reactions in type-II nodal-line topological catalyst Mg₃Bi₂

Min Zhao, Weizhen Meng,* Lirong Wang, Zeqing He, Lei Jin, Ying Liu, Xuefang Dai, Xiaoming Zhang,* Hongshi Li* and Guodong Liu*

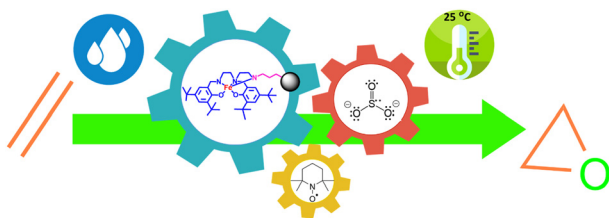
26575



Molecular torsion controls the excited state relaxation pathways of multibranch tetraphenylpyrazines: effect of substitution of morpholine vs. phenoxazine

Hasim Fayiz Pananilath, Chinju Govind, Tessa D. Thadathilanickal and Venugopal Karunakaran*

26588



TEMPO and a co-reductant mediated aerobic epoxidation of olefins using a new magnetically recoverable iron(III) bis(phenol)diamine complex: experimental and computational studies

Pegah Mohammadpour, Elham Safaei,* Elham Mazarei and Constantinos D. Zeinalipour-Yazdi

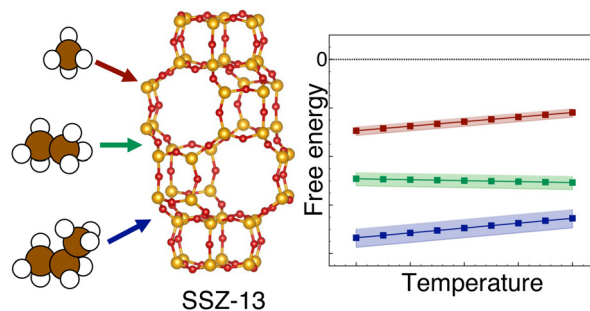


RESEARCH PAPERS

26604

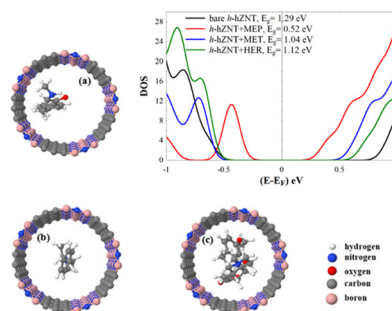
Free and internal energies for the adsorption of short alkanes into the zeolite SSZ-13 from *ab initio* molecular dynamics simulations

Daniel J. Hutton and Florian Göttl*

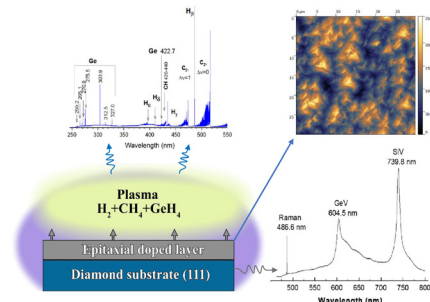


26613

Towards nanotube-based sensors for discrimination of drug molecules

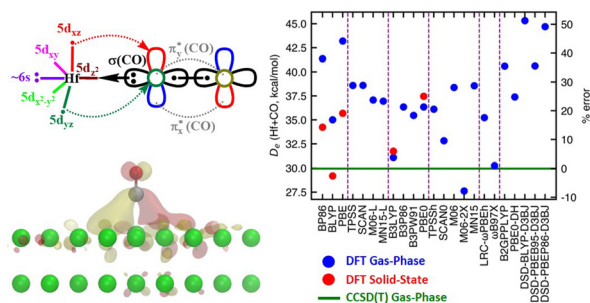
Laith A. Algharagholy, Víctor M. García-Suárez,*
Ohood Abdullah Albeydani and Jehan Alqahtani

26623

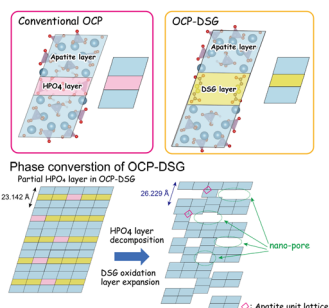
In situ doping of epitaxial diamond with germanium by microwave plasma CVD in GeH₄-CH₄-H₂ mixtures with optical emission spectroscopy monitoringVladimir Yurov,* Andrey Bolshakov, Victor Ralchenko,*
Irina Fedorova, Artem Martyanov, Pavel Pivovarov,
Vladimir Artemov, Andrew Khomich, Roman Khmelniyskiy
and Kirill Boldyrev

26632

Gas-phase and solid-state electronic structure analysis and DFT benchmarking of HfCO

Isuru R. Ariyaratna, Yeongsu Cho, Chenru Duan and
Heather J. Kulik*

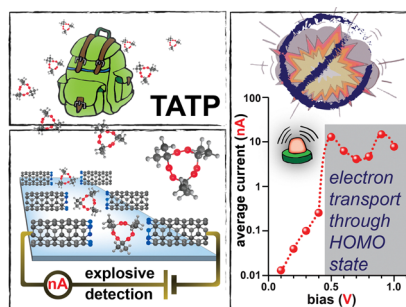
26640



Interlayer expansion of octacalcium phosphate via forced oxidation of the intercalated molecules within its interlayers

Yuki Sugiura,* Etsuko Yamada and Masanori Horie

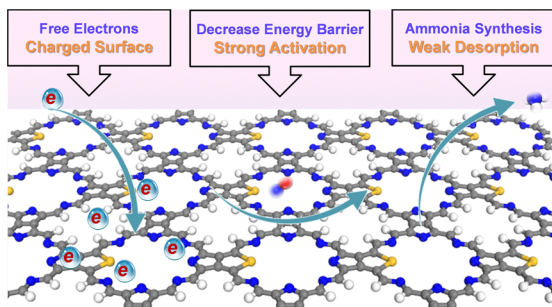
26648



Tunnel junction sensing of TATP explosive at the single-molecule level

Aleksandar Ž. Tomović, Helena Miljković, Miloš S. Dražić, Vladimir P. Jovanović and Radomir Zikić*

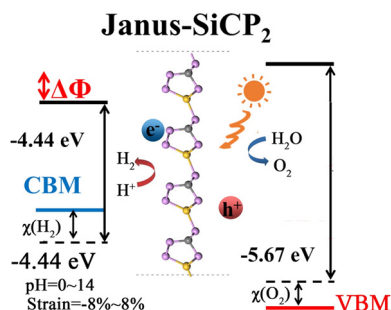
26659



Theoretical insight into the essential role of charged surface for ammonia synthesis: Si-decorated carbon nitride electrode

Lei Yang, Jiake Fan and Weihua Zhu*

26666



Metal-free Janus α - and β -SiCP₄: designing stable and efficient two-dimensional semiconductors for water splitting

Yanfu Zhao, Bofeng Zhang* and Jiahe Lin*

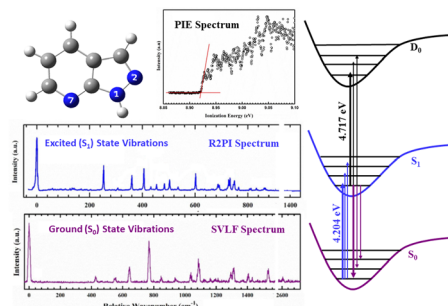


RESEARCH PAPERS

26679

Laser spectroscopic characterization of supersonic jet cooled 2,7-diazaindole

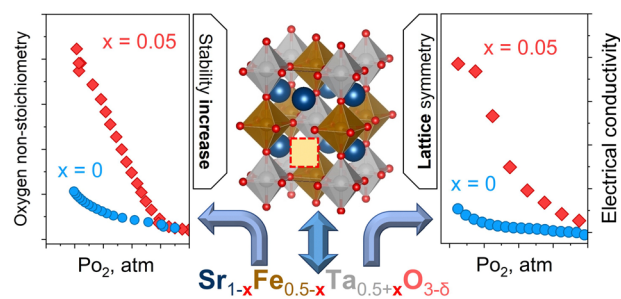
Simran Baweja, Bhavika Kalal and Surajit Maity*



26692

The influence of strontium deficiency on thermodynamics of defect formation, structural stability and electrical transport of $\text{SrFe}_{0.5}\text{Ta}_{0.5}\text{O}_{3-\delta}$ -based solid solutions with an excess tantalum content

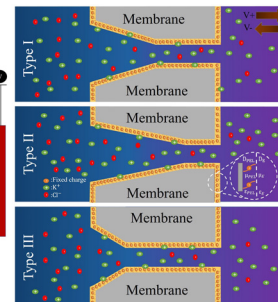
B. V. Politov,* J. C. Waerenborgh, I. R. Shein and O. V. Merkulov



26716

Smart nanochannels: tailoring ion transport properties through variation in nanochannel geometry

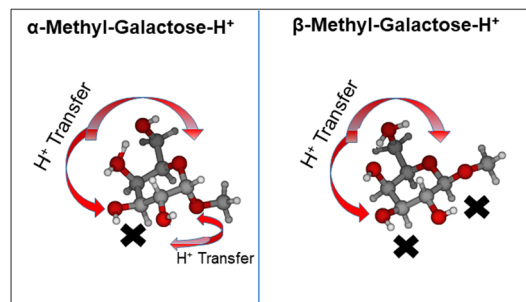
Amirhossein Heydari, Mahdi Khatibi and Seyed Nezameddin Ashrafizadeh*



26737

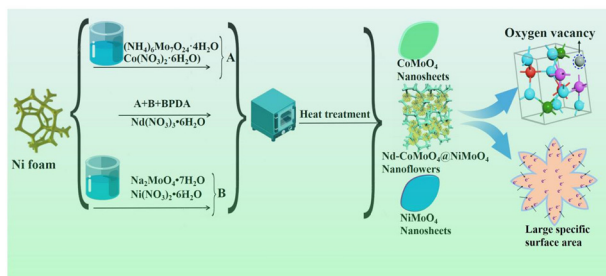
Selective reactivity of glycosyl cation stereoisomers: the role of intramolecular hydrogen bonding

M. P. Dvores,* P. Çarçabal and R. B. Gerber*



RESEARCH PAPERS

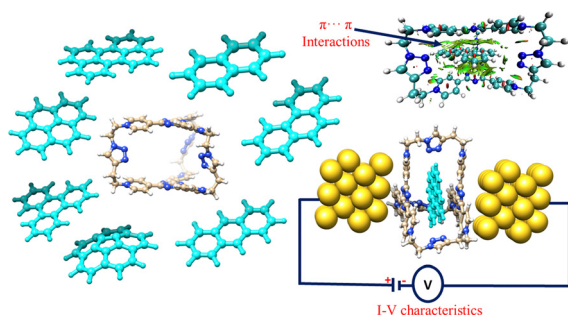
26748



Coupling of Nd doping and oxygen-rich vacancy in $\text{CoMoO}_4@NiMoO_4$ nanoflowers toward advanced supercapacitors and photocatalytic degradation

Jing Wang,* Gang Wang, Shen Wang, Tingting Hao and Jian Hao

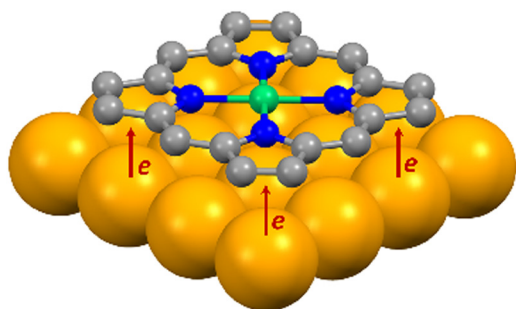
26767



Exploring $\pi-\pi$ interactions and electron transport in complexes involving a hexacationic host and PAH guest: a promising avenue for molecular devices

Haobam Kisan Singh, Upasana Nath, Niharika Keot and Manabendra Sarma*

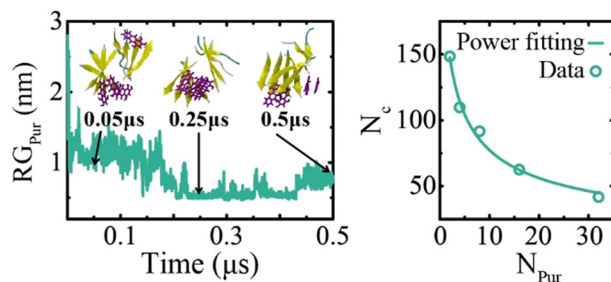
26779



A local point of view of the $\text{Cu}(100) \rightarrow \text{NiTPP}$ charge transfer at the NiTPP/Cu(100) interface

Silvia Carlotto, Alberto Verdini,* Giovanni Zamborlini, Iulia Cojocariu, Vitaliy Feyar, Luca Floreano and Maurizio Casarin*

26787



Dose-dependent binding behavior of anthraquinone derivative purpurin interacting with tau-derived peptide protofibril

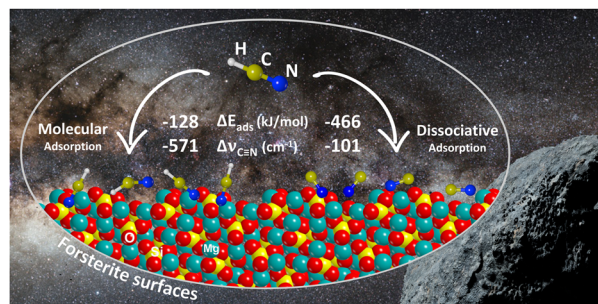
Xiaoxiao Wu, Lili Zhu, Gang Wang, Qingwen Zhang and Zhenyu Qian*



26797

Adsorption of HCN on cosmic silicates: a periodic quantum mechanical study

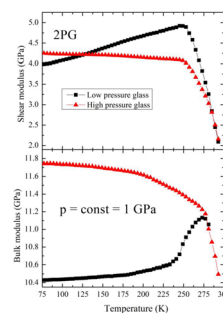
Niccolò Bancone, Stefano Pantaleone, Piero Ugliengo, Albert Rimola* and Marta Corno*



26813

Thermobaric history as a tool to govern properties of glasses: case of dipropylene glycol

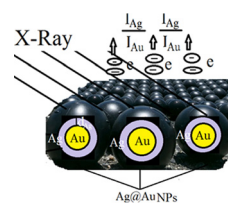
Igor Danilov,* Elena Gromnitskaya and Vadim Brazhkin



26820

A simple equation to determine the shell thicknesses of core-shell nanoparticles based on XPS data of their elemental composition

Alexey T. Kozakov,* Anton A. Skriabin and Niranjana Kumar



Ag@Au NPs

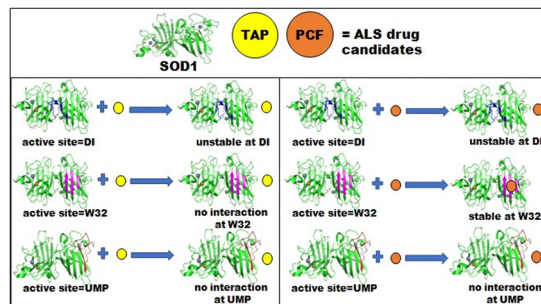
$$d_{Ag} = \lambda_{Au}^{Ag} \cdot \ln \left(1 + \frac{I_{Au}}{I_{Ag}} \cdot \frac{\lambda_{Au}^{Au}}{\lambda_{Au}^{Ag} + \lambda_{Au}^{Au}} \cdot \frac{I_{Ag}}{I_{Au}} \right)$$

A simple equation is obtained for determining the shell thickness of core-shell nanoparticles based on XPS data

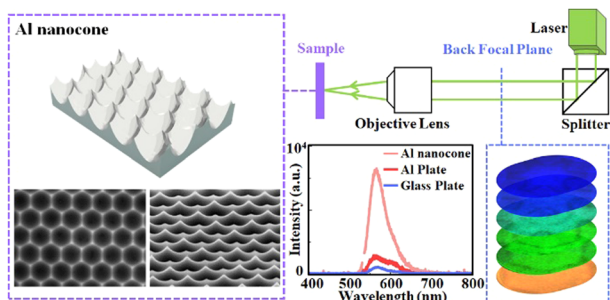
26833

In silico analysis of SOD1 aggregation inhibition modes of tertiary amine pyrazolone and pyrano coumarin ferulate as ALS drug candidates

Aziza Rahman, Bondeepa Saikia and Anupaul Baruah*



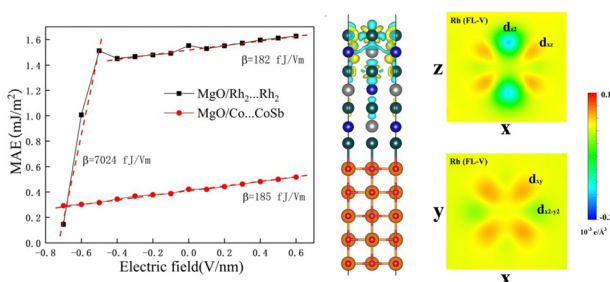
26847



Surface lattice resonances enhanced directional amplified spontaneous emission on plasmonic honeycomb nanocone array

Dongda Wu, Yi Wang,* Jiamin Xiao, Jiang Hu, Xuchao Zhao, Yuhao Gao, Jiazhi Yuan and Wenxin Wang*

26853

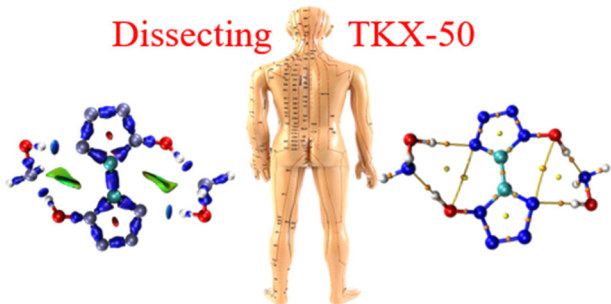


Giant unilateral electric-field control of magnetic anisotropy in MgO/Rh₂CoSb heterojunctions

Shiming Yan, Yue Hu, Deyou Jin, Ru Bai, Wen Qiao* and Tiejun Zhou*

26861

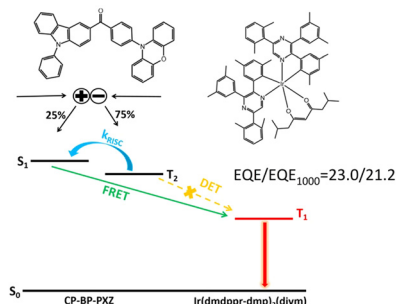
Dissecting TKX-50



Theoretical study on intra-molecule interactions in TKX-50

Chunhai Yang,* Xue Li,* Ning Zhou, Huitong Dong,* Xiuli Hu, Junxun Jin, Tao Huang and Jinhui Wang

26878



Exciton dynamics of an aggregation-induced delayed fluorescence emitter in non-doped OLEDs and its application as host for high-efficiency red phosphorescent OLEDs

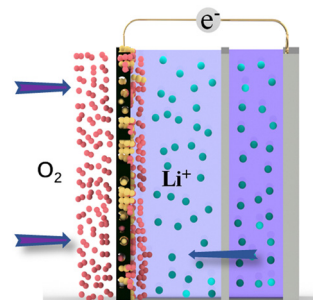
Hanlin Li, Chengwei Lin, Yibing Wu, Xianfeng Qiao, Dezhi Yang, Yanfeng Dai, Qian Sun, Tansir Ahamad, Zhujin Zhao* and Dongge Ma*



26885

Cobalt-doped tin disulfide catalysts for high-capacity lithium–air batteries with high lifetime

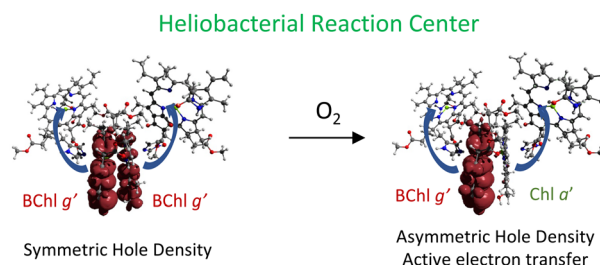
Jie Li, Yuzhi Shi, Junhai Wang, Qianhe Liu, Lihua Luan, Qiang Li, Qinghao Cao, Tianyu Zhang and Hong Sun*



26894

Electronic structure and energetics of a heterodimeric BChl *g'*/Chl *a'* special pair generated by exposure of *Heliomicrobium modesticaldum* to dioxygen

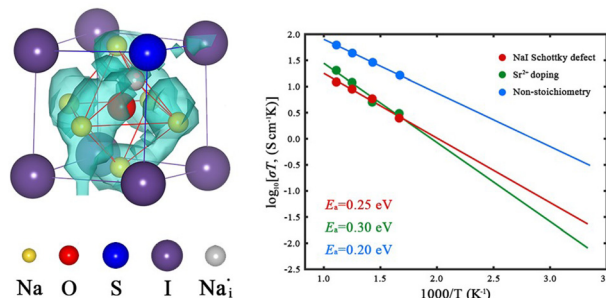
Divya Kaur,* Bryan Ferlez, Patrick Landry, Till Biskup, Stefan Weber, John H. Golbeck,* K. V. Lakshmi* and Art van der Est*



26906

Investigation of the sodium-ion transport mechanism and elastic properties of double anti-perovskite $\text{Na}_3\text{S}_{0.5}\text{O}_{0.5}\text{I}$

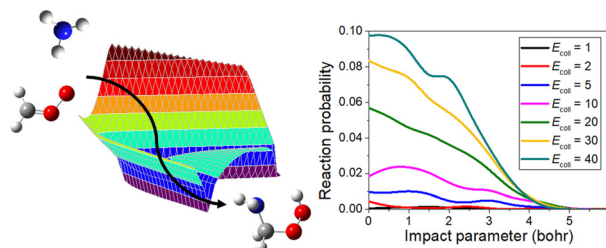
Sen Lian, Congcong Li, Chen Kang, Junfeng Ren and Meina Chen*



26917

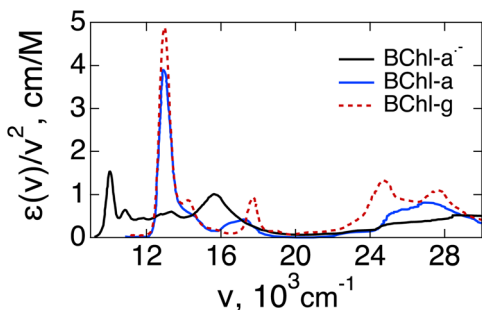
Full-dimensional automated potential energy surface development and detailed dynamics for the $\text{CH}_2\text{OO} + \text{NH}_3$ reaction

Cangtao Yin* and Gábor Czakó*



COMMENT

26923



Comment on "Applicability of perturbed matrix method for charge transfer studies at bio/metallic interfaces: a case of azurin" by O. Kontkanen, D. Biriukov and Z. Futera, *Phys. Chem. Chem. Phys.*, 2023, 25, 12479

Setare Mostajabi Sarhangi and Dmitry V. Matyushov*

CORRECTION

26929

Correction: Induced UV photon sensing properties in narrow bandgap CdTe quantum dots through controlling hot electron dynamics

Thankappan Thrupthika, Devaraj Nataraj,* Subramaniam Ramya, Arumugam Sangeetha and T. Daniel Thangadurai

