PCCP

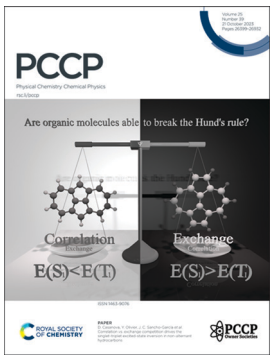
Physical Chemistry Chemical Physics – An international journal

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

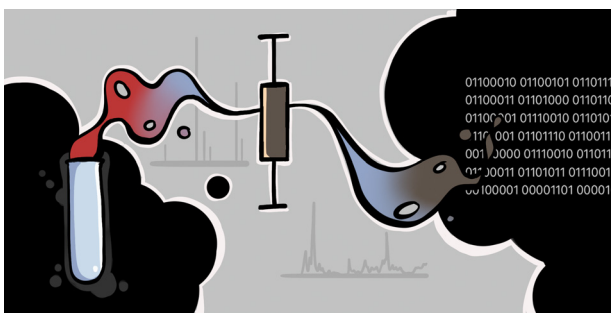
ISSN 1463–9076 CODEN PPCPFQ 25(39) 26399–26932 (2023)



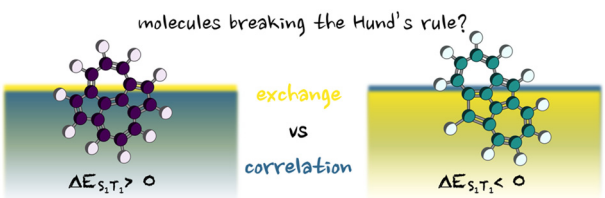
Cover
See D. Casanova, Y. Olivier, J. C. Sancho-García *et al.*, pp. 26417–26428. Image reproduced by permission of Gaetano Ricci from *Phys. Chem. Chem. Phys.*, 2023, **25**, 26417.

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



RESEARCH PAPERS



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.

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.

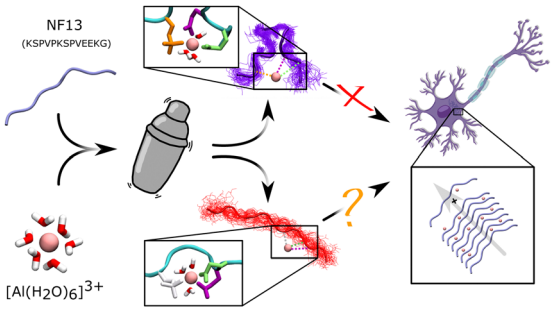
Information for Authors

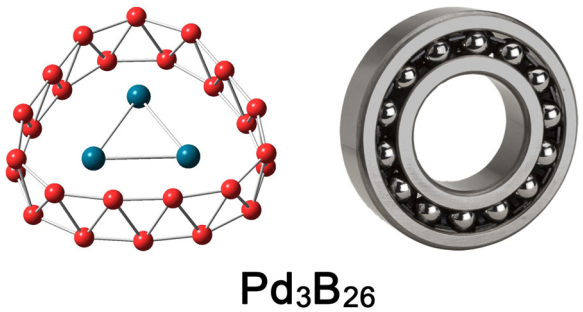
Full details on how to submit material for publication in PCCP are given in the Instructions for Authors (available from **http://www.rsc.org/authors**). Submissions should be made via the journal's **homepage: rsc.li/pccp**

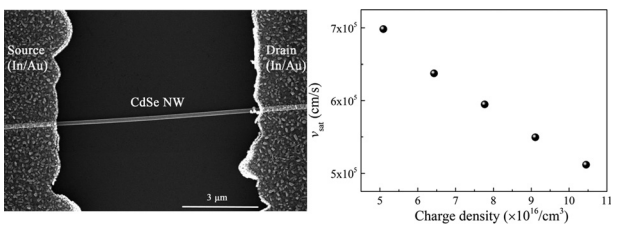
♾ The paper used in this publication meets the requirements of ANSI/NISO Z39.48–1992 (Permanence of Paper).

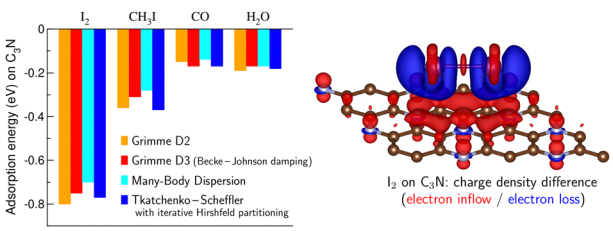
Registered charity number: 207890

RESEARCH PAPERS



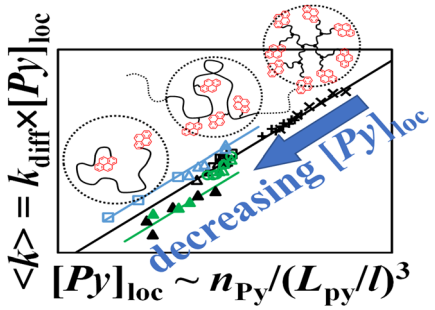


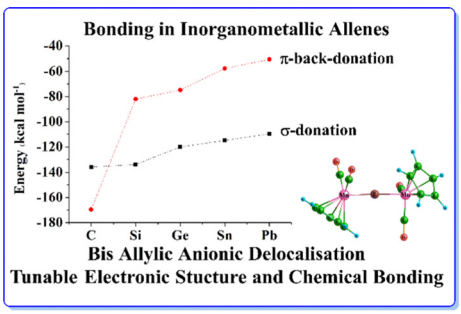


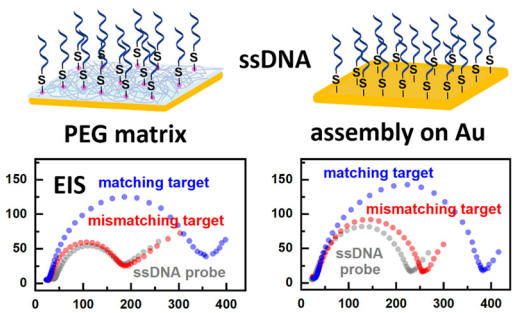


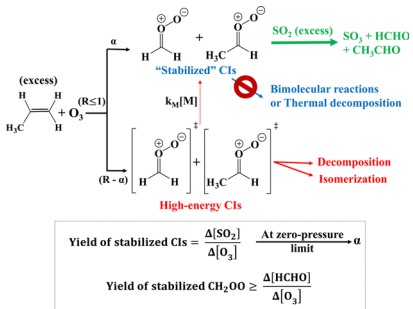
RESEARCH PAPERS

RESEARCH PAPERS



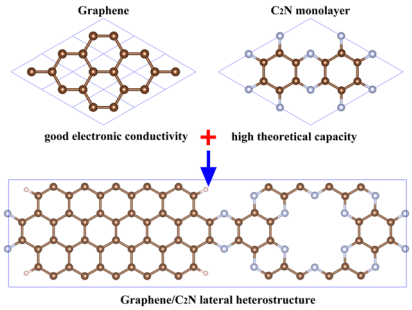






RESEARCH PAPERS

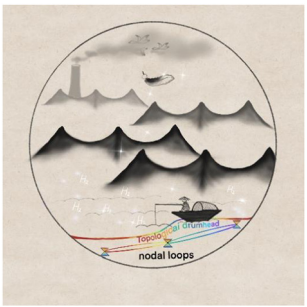
26557



Graphene/C_2N lateral heterostructures as promising anode materials for lithium-ion batteries

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

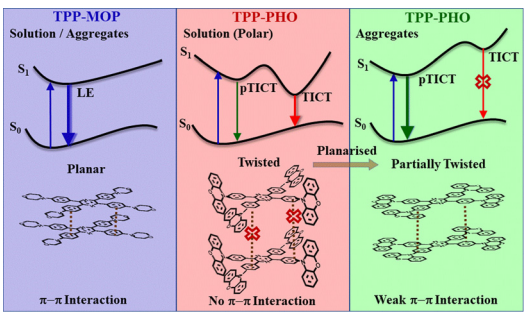
26566



Drumhead surface states promoted hydrogen evolution reactions in type-II nodal-line topological catalyst Mg_3Bi_2

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

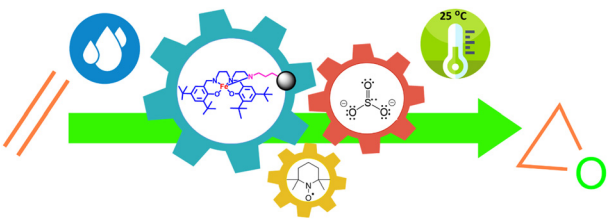
26575



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

Hasim Fayiz Pananilath, Chinju Govind, Tessy 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

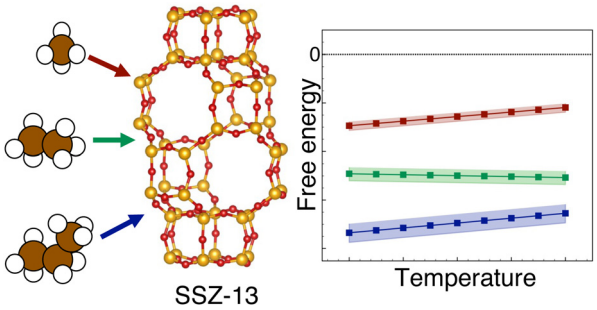
Pegah Mohammadpour, Elham Safaei,* Elham Mazarei and Constantinos D. Zeinalipour-Yazdi

RESEARCH PAPERS

26604

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

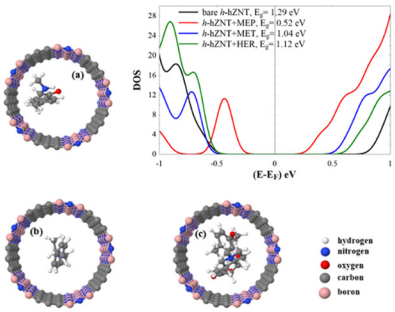
Daniel J. Hutton and Florian Göltl*



26613

Towards nanotube-based sensors for discrimination of drug molecules

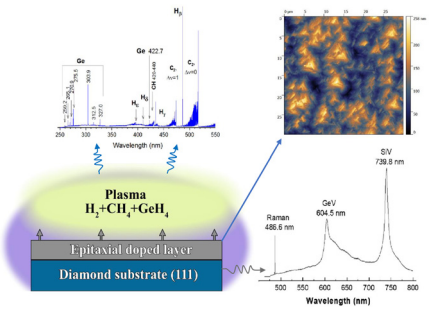
Laith A. Algharagholy, Víctor M. García-Suárez,* Ohood Abdullah Albeydani and Jehan Alqahtani



26623

In situ doping of epitaxial diamond with germanium by microwave plasma CVD in GeH_4–CH_4–H_2 mixtures with optical emission spectroscopy monitoring

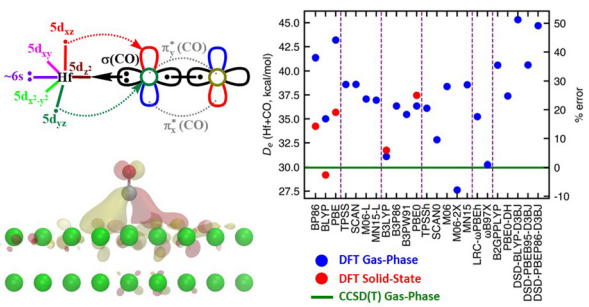
Vladimir Yurov,* Andrey Bolshakov, Victor Ralchenko,* Irina Fedorova, Artem Martyanov, Pavel Pivovarov, Vladimir Artemov, Andrew Khomich, Roman Khmelnitskiy and Kirill Boldyrev



26632

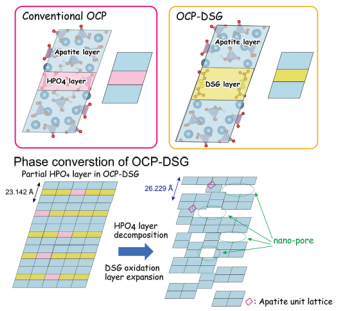
Gas-phase and solid-state electronic structure analysis and DFT benchmarking of HfCO

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



RESEARCH PAPERS

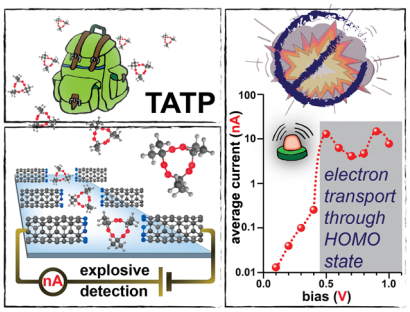
26640



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

Yuki Sugiura,* Etsuko Yamada and Masanori Horie

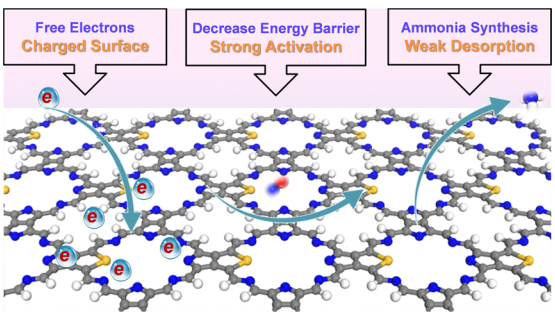
26648



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

Aleksandar Ž. Tomović, Helena Miljkovic, Miloš S. Dražić, Vladimir P. Jovanović and Radomir Zikic*

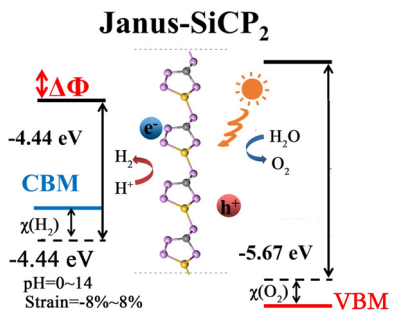
26659



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

Lei Yang, Jiake Fan and Weihua Zhu*

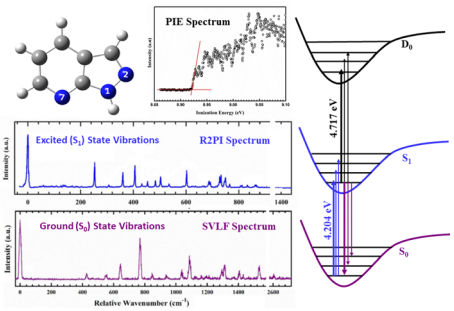
26666

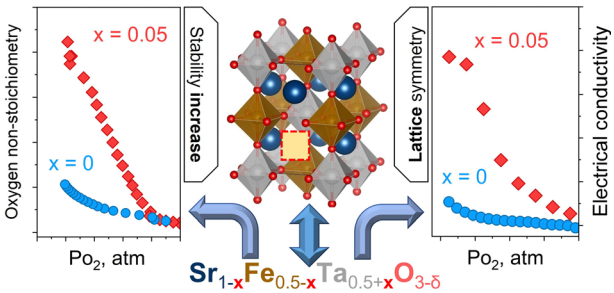


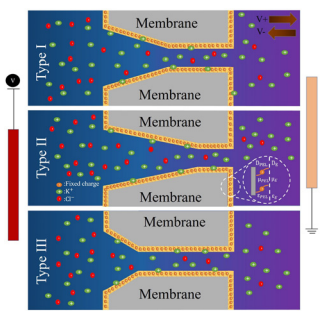
Metal-free Janus α- and β-$SiCP_4$: designing stable and efficient two-dimensional semiconductors for water splitting

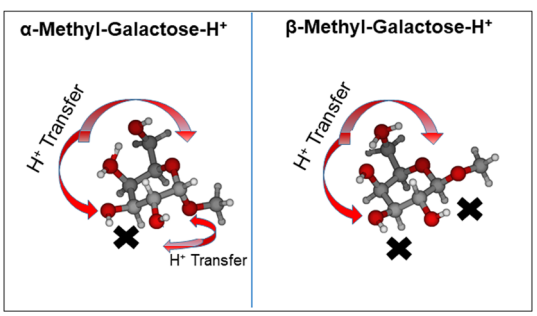
Yanfu Zhao, Bofeng Zhang* and Jiahe Lin*

RESEARCH PAPERS

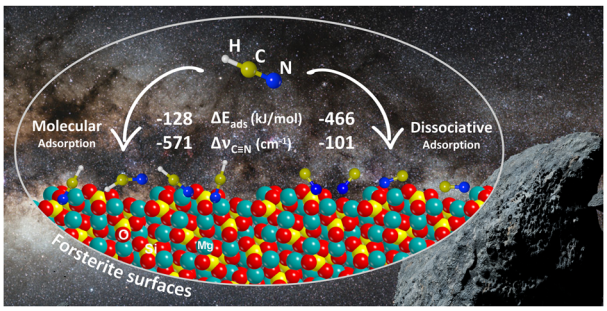


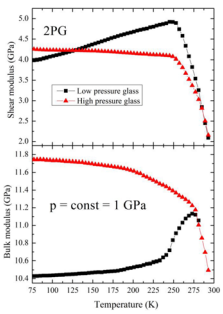


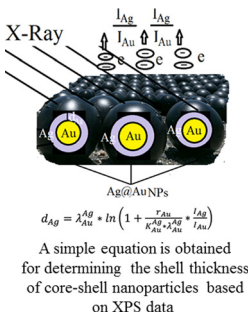


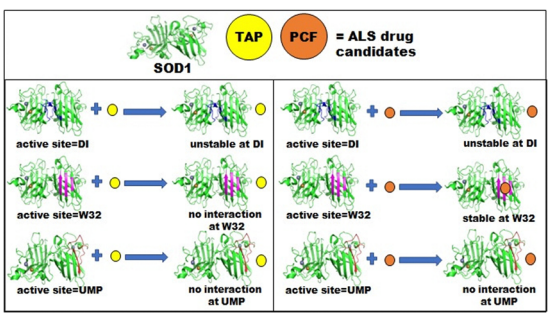


RESEARCH PAPERS



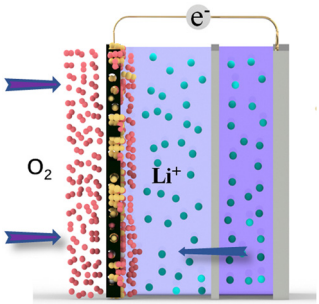


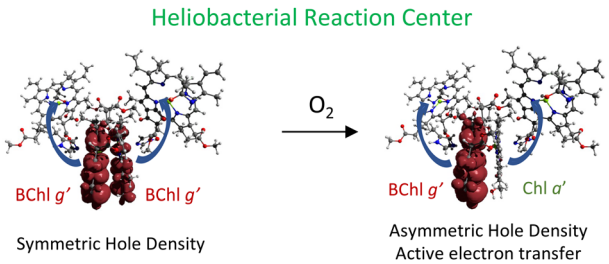


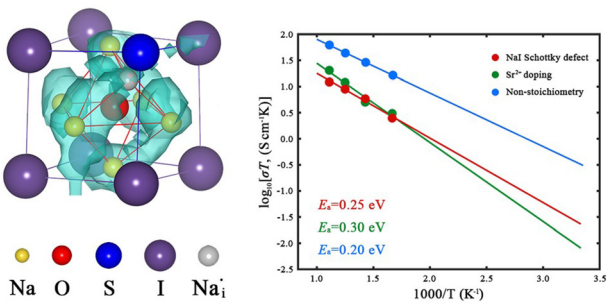


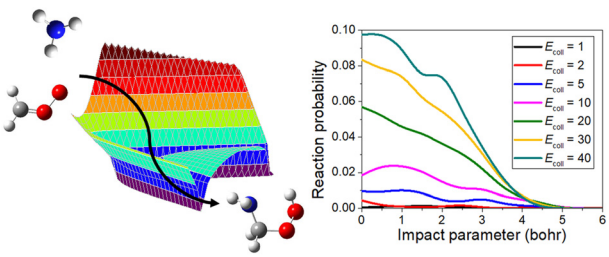
RESEARCH PAPERS

RESEARCH PAPERS

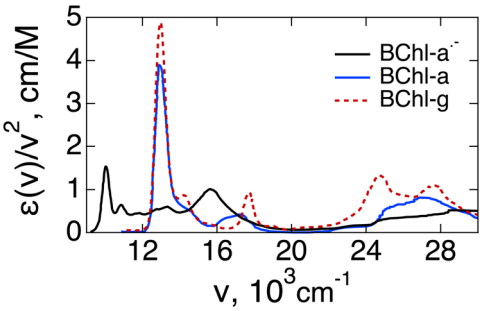








COMMENT



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

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