PCCP

Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

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

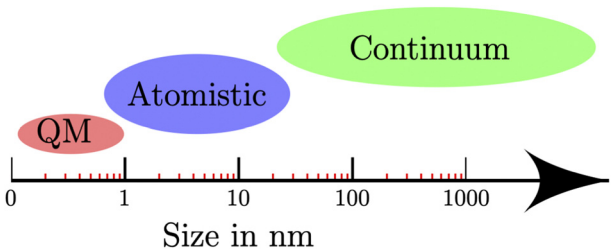
IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 26(37) 24193–24718 (2024)

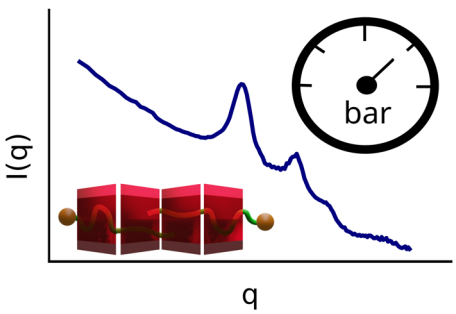
Cover
See Yoshiaki Kawagoe *et al.*, pp. 24250–24260. Image reproduced by permission of Yoshiaki Kawagoe from *Phys. Chem. Chem. Phys.*, 2024, **26**, 24250.

Inside cover
See Larissa dos Santos Silva Araújo and Leonardo Chiappisi, pp. 24246–24249. Image reproduced by permission of Institut Laue-Langevin from *Phys. Chem. Chem. Phys.*, 2024, **26**, 24246. Elephants by Patryk Kosmider via Adobe Stock.

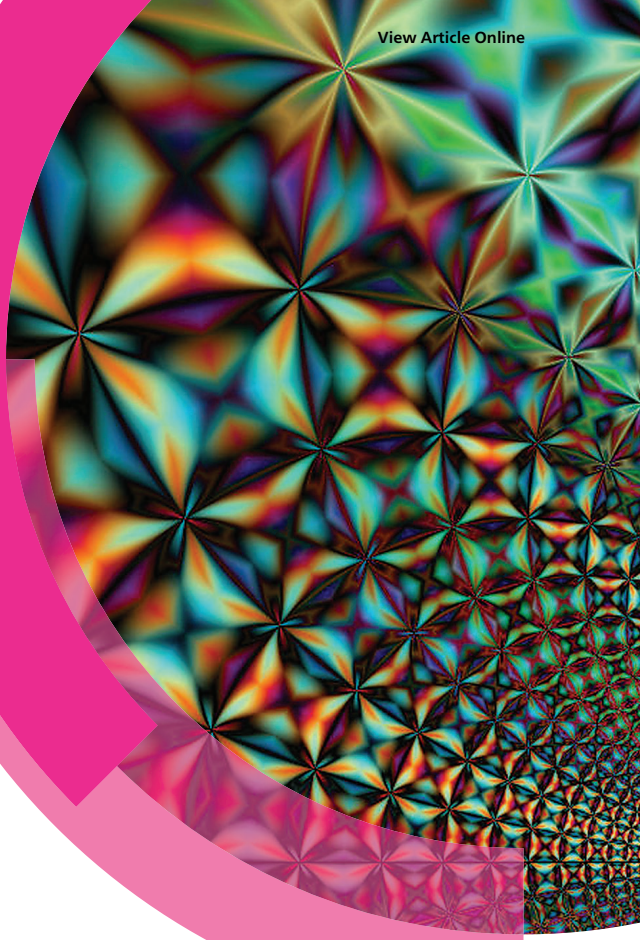
REVIEW



COMMUNICATION



ROYAL SOCIETY OF CHEMISTRY



RSC Advances

At the heart of open access for the global chemistry community

Editor-in-chief

Russell J Cox
Leibniz Universität Hannover, Germany

We stand for:

Breadth We publish work in all areas of chemistry and reach a global readership

Affordability Low APCs, discounts and waivers make publishing open access achievable and sustainable

Quality Research to advance the chemical sciences undergoes rigorous peer review for a trusted, society-run journal

Community Led by active researchers, we publish quality work from scientists at every career stage, and all countries

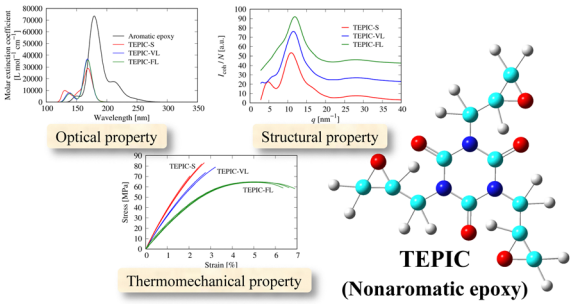
Submit your work now

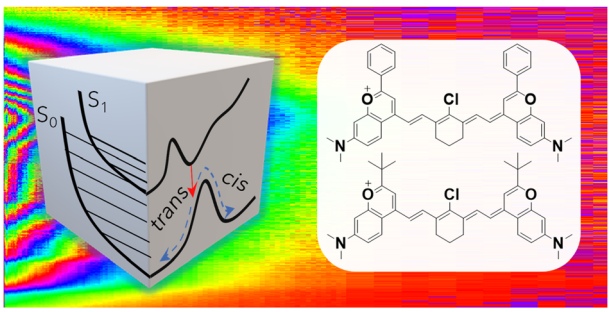
rsc.li/rsc-advances

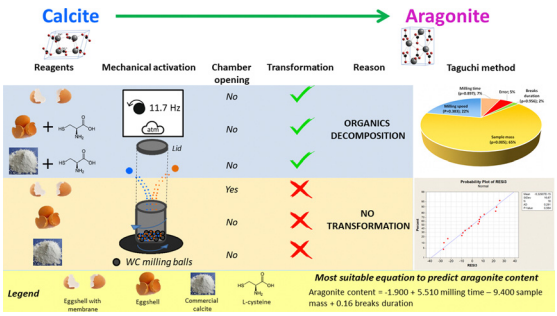
@RSC_Adv

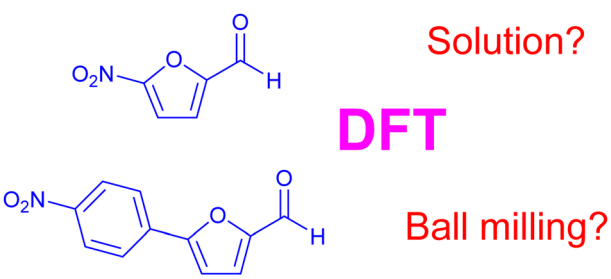
Registered charity number: 207890

RESEARCH PAPERS



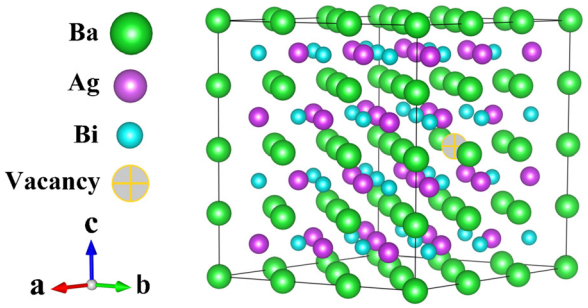


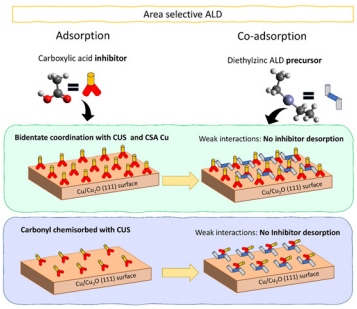


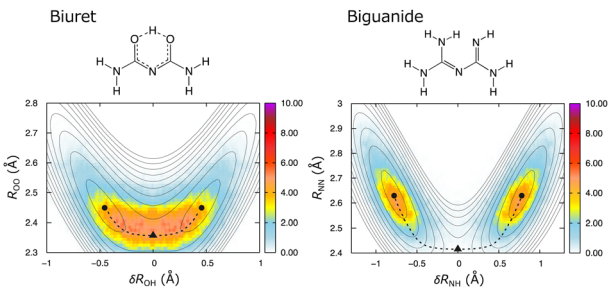


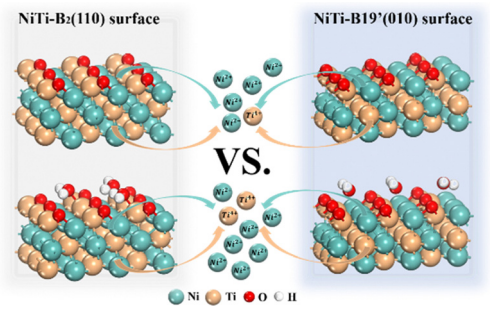
RESEARCH PAPERS

RESEARCH PAPERS



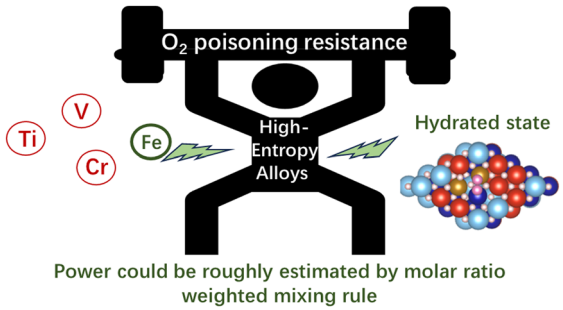






RESEARCH PAPERS

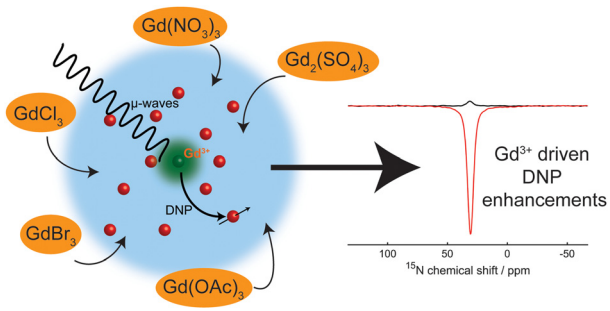
24384



Theoretical study on the surface poisoning of high-entropy alloys during hydrogen storage cycles: the effect of metal elements and phases

Ming Jiang, Yixin Yang, Hongjiao Li* and Bin Liang

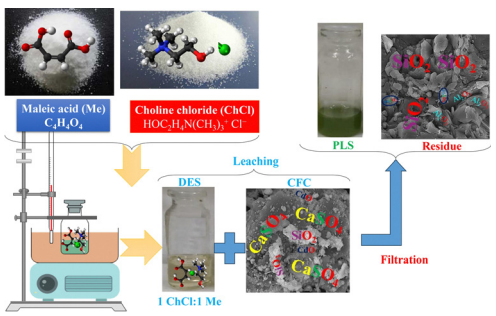
24395



Optimisation of dynamic nuclear polarisation using "off-the-shelf" Gd(III)-based polarising agents

Daniel J. Cheney, Paolo Cerreia Vioglio, Adam Brookfield and Frédéric Blanc*

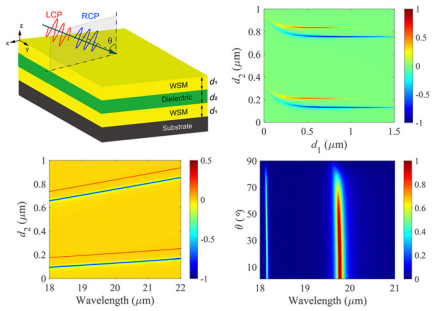
24407



Green leaching of cold filter cakes using choline chloride–maleic acid deep eutectic solvent and molecular dynamics simulation

Bahram Behnajady,* Matin Najafi and Saeid Karimi*

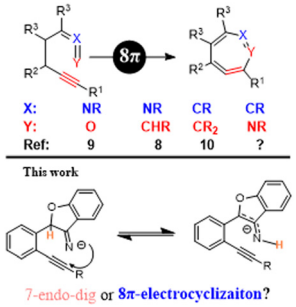
24423

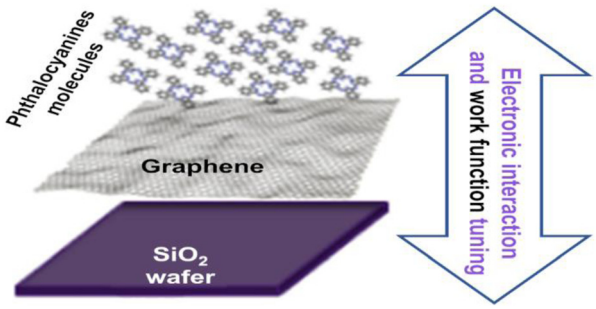


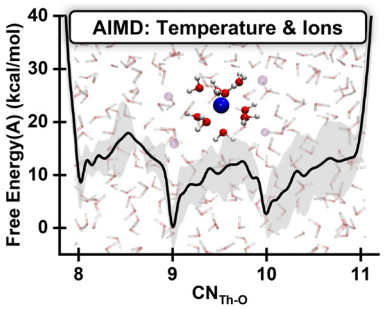
Weyl semimetal/dielectric/Weyl semimetal stack for highly circularly polarized thermal radiation

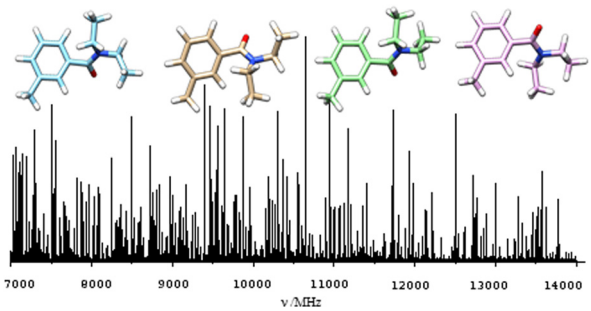
Xin Cui, Qi Fang, Liming Qian and Gaige Zheng*

RESEARCH PAPERS



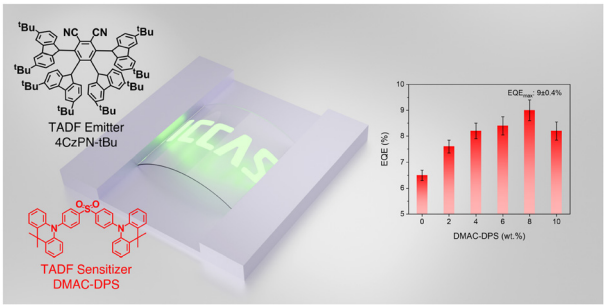


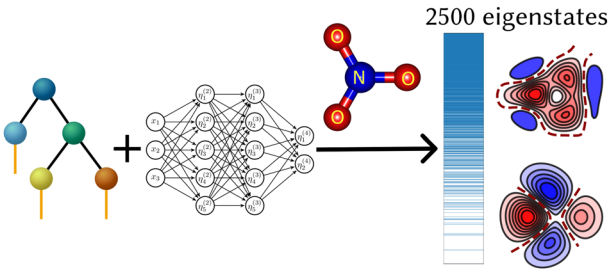


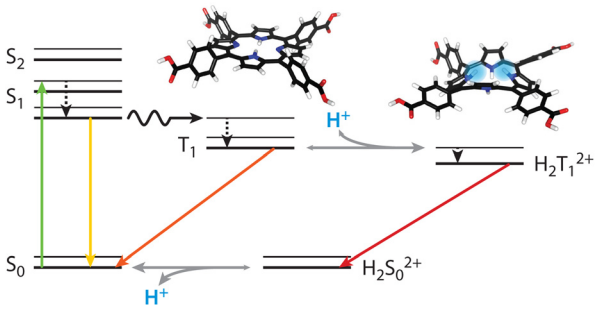


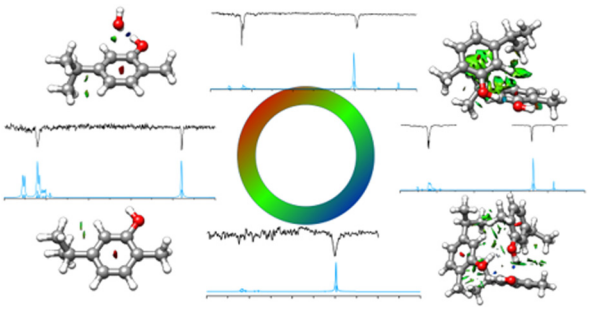
RESEARCH PAPERS

RESEARCH PAPERS



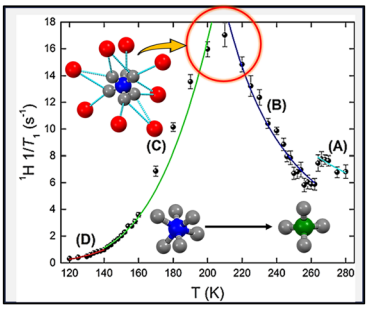


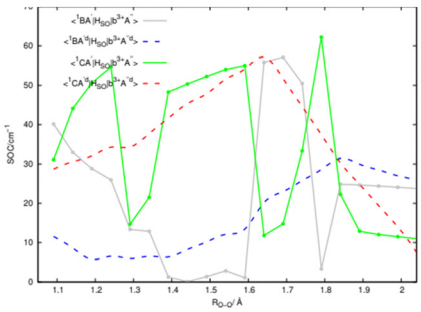


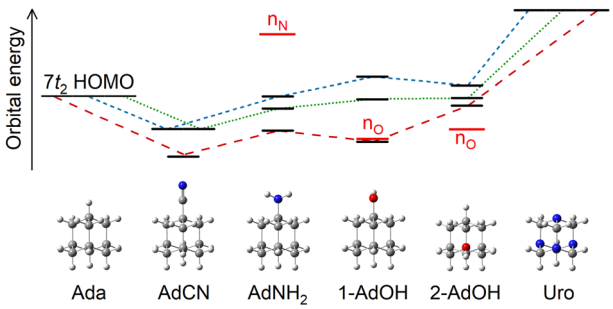


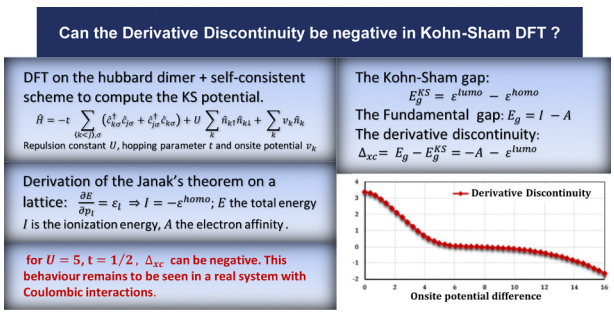
RESEARCH PAPERS

RESEARCH PAPERS



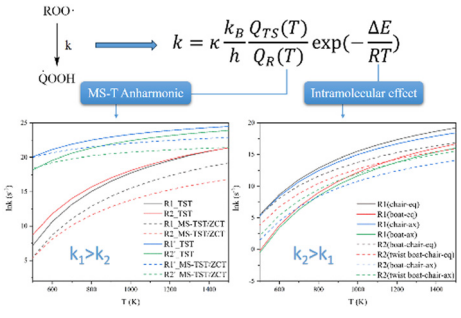


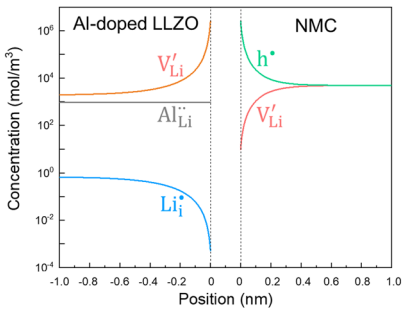


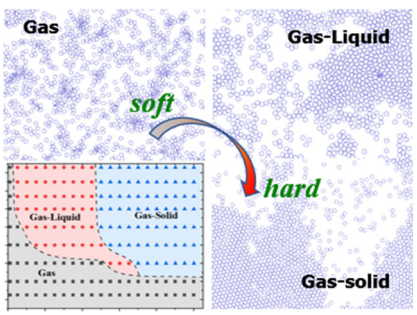


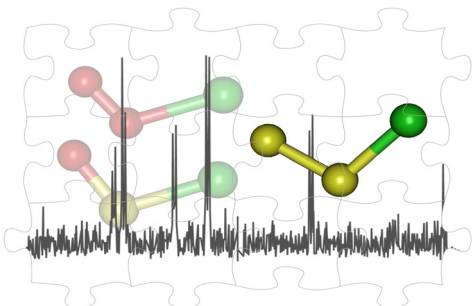
RESEARCH PAPERS

RESEARCH PAPERS









CORRECTIONS

24714

Correction: The Lennard-Jones potential: when (not) to use it

Xipeng Wang, Simón Ramírez-Hinestrosa, Jure Dobnikar and Daan Frenkel*

24716

Correction: Water adsorption lifts the (2 × 1) reconstruction of calcite(104)

Jonas Heggemann, Simon Aeschlimann, Tobias Dickbreder, Yashasvi S. Ranawat, Ralf Bechstein, Angelika Kühnle, Adam S. Foster* and Philipp Rahe*