PCCP

Physical Chemistry Chemical Physics – An international journal

rsc.li/pccp

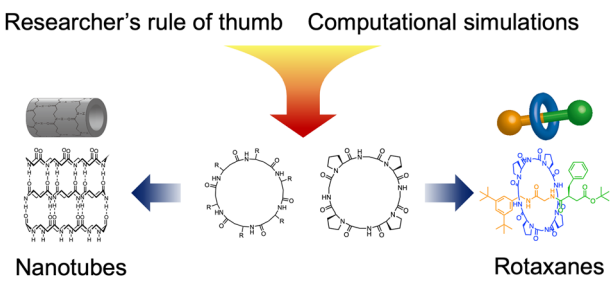
The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

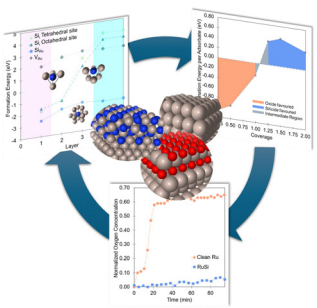
ISSN 1463–9076 CODEN PPCPFQ 26(46) 28763–29168 (2024)

Cover
See Kazuki Nakamura *et al.*, pp. 28800–28807. Image reproduced by permission of Ryoto Yabuta, Norihisa Kobayashi and Kazuki Nakamura from *Phys. Chem. Chem. Phys.*, 2024, **26**, 28800.

REVIEW



COMMUNICATION



ROYAL SOCIETY OF CHEMISTRY

Environmental Science: Atmospheres

GOLD OPEN ACCESS

Connecting communities and inspiring new ideas

rsc.li/submittoEA

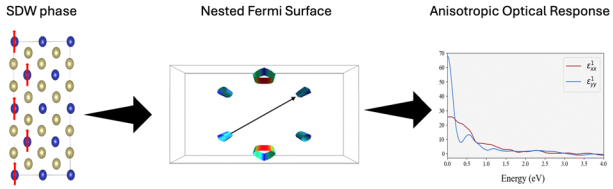
Fundamental questions
Elemental answers

Registered charity number: 207890

RESEARCH PAPERS

RESEARCH PAPERS

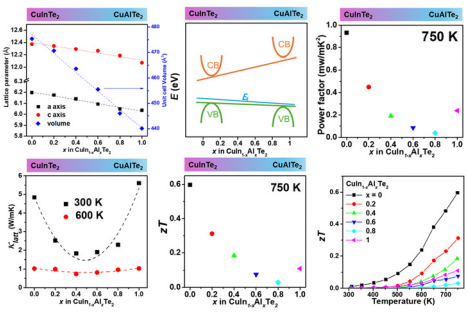
28849



Magnetic stability, Fermi surface topology, and spin-correlated dielectric response in monolayer 1T-$CrTe_2$

Ahmed Elrashidy* and Jia-An Yan

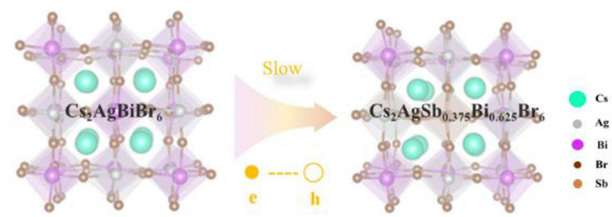
28858



Significant reduction of lattice thermal conductivity observed in $CuInTe_2$–$CuAlTe_2$ solid-solution alloys

Seungchan Seon, BeomSoo Kim, Okmin Park, Hyungyu Cho and Sang-il Kim*

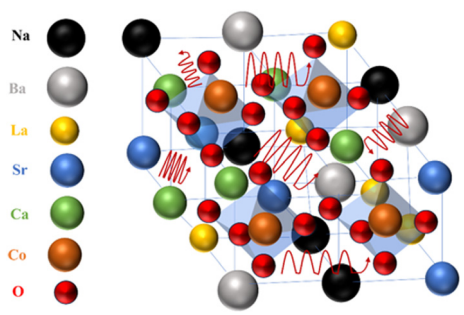
28865



Effect of Sb–Bi alloying on electron–hole recombination time of $Cs_2AgBiBr_6$ double perovskite

Yuzhuo Lv, Chang Liu, Yuhang Ma, Guodong Liu, Fei Wang, Yuhong Xia, Chundan Lin, Changjin Shao and Zhenqing Yang*

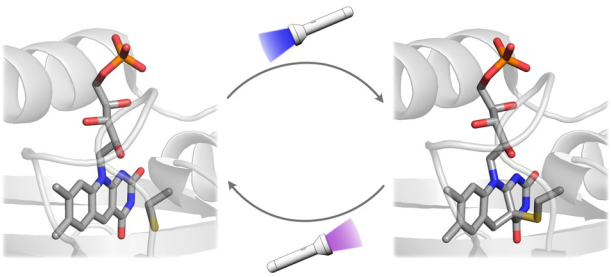
28874

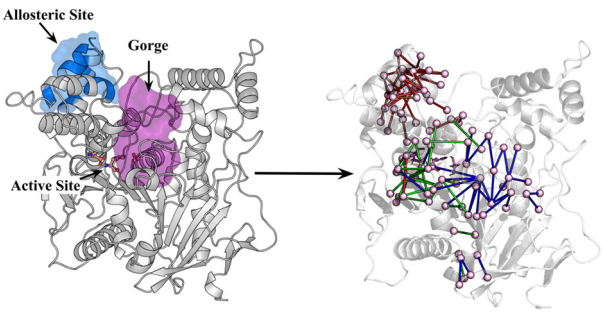


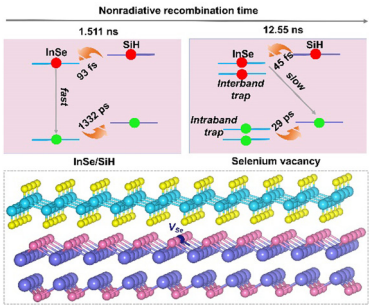
Thermoelectric behavior of $(Ba_{0.2}Sr_{0.2}Ca_{0.2}La_{0.2}Na_{0.2})CoO_3$ high entropy cobaltate-based perovskite

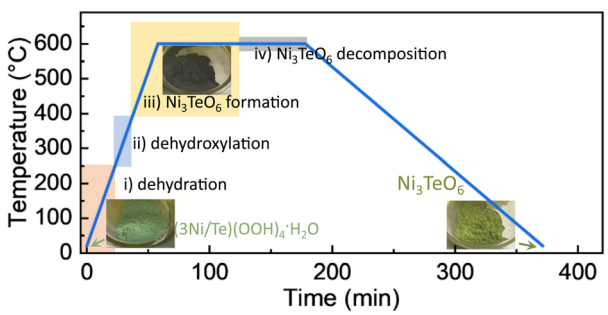
Tathagata Bhattacharya, Ritwik Banerjee and Tanmoy Maiti*

RESEARCH PAPERS









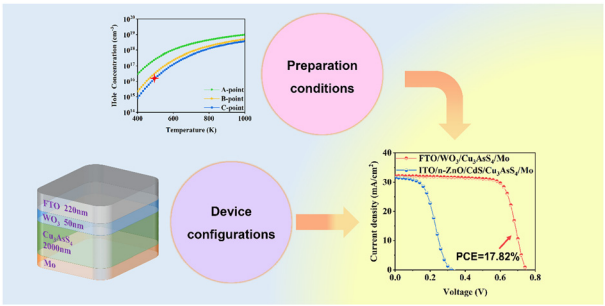
RESEARCH PAPERS

RESEARCH PAPERS

28958

Optimization of preparation conditions and design of device configurations for Cu_3AsS_4 solar cells: a combined study of first-principles calculations and SCAPS-1D device simulations

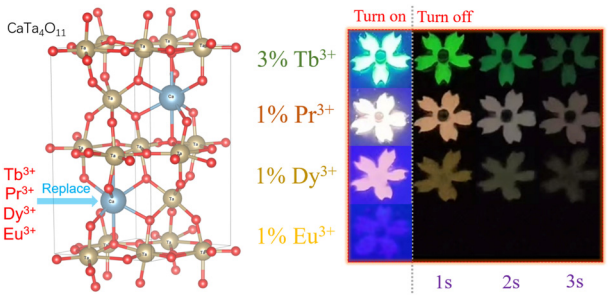
Yi Huang, Changqing Lin, Yang Xue, Binyuan Huang and Dan Huang*



28971

Molten salt synthesized Tb^{3+}, Pr^{3+} or Dy^{3+} single doped $CaTa_4O_{11}$ with persistent luminescence

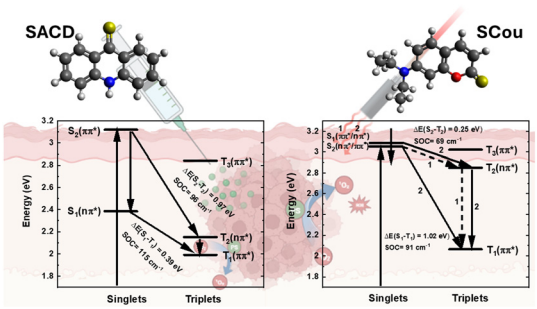
Yuhan Fan, Yongze Cao,* Meiling Li, Sai Xu, Yichao Wang, Xizhen Zhang, Jinsu Zhang and Baojiu Chen*



28980

Electronic relaxation pathways in thio-acridone and thio-coumarin: two heavy-atom-free photosensitizers absorbing visible light

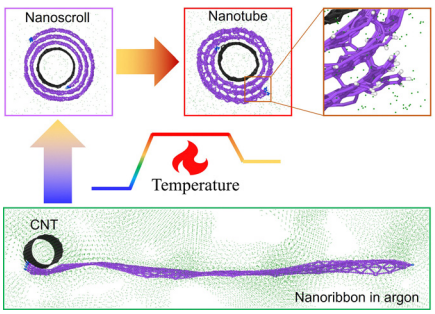
Chris Acquah, Sean Hoehn, Sarah Krul, Steffen Jockusch, Shudan Yang, Sourav Kanti Seth, Eric Lee, Han Xiao and Carlos E. Crespo-Hernández*



28992

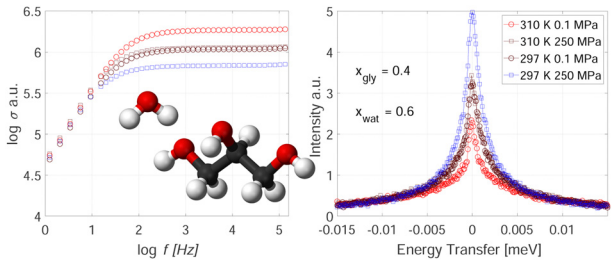
An annealing approach to form a nanotube from graphdiyne ribbon: a theoretical prediction

Bo Song, Kun Cai,* Jiao Shi and Qing-Hua Qin*



RESEARCH PAPERS

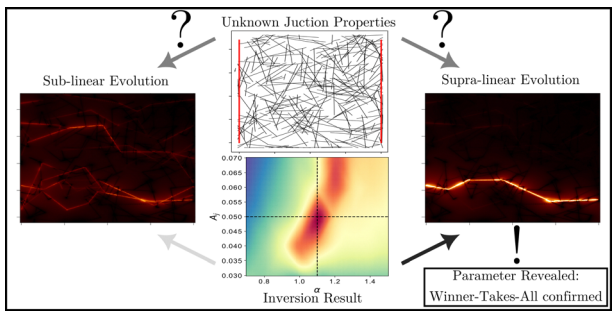
29003



Density scaling and isodynes in glycerol–water mixtures

David B. Noirat, Bernhard Frick, Bo Jakobsen, Markus Appel and Kristine Niss*

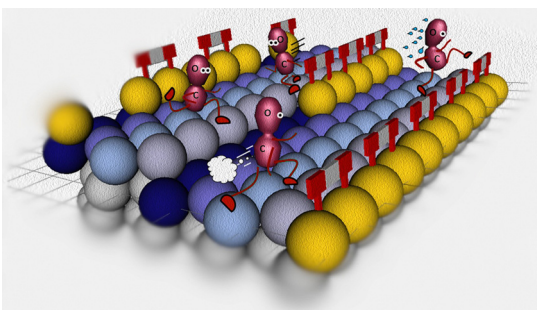
29015



Identifying winner-takes-all emergence in random nanowire networks: an inverse problem

F. R. Duarte,* S. Mukim, M. S. Ferreira and C. G. Rocha

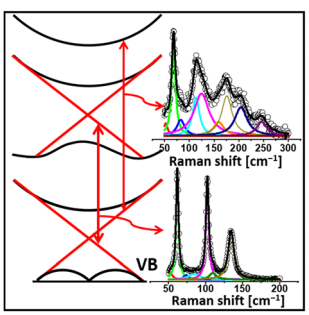
29027



The decisive role of Au in CO diffusion on Pt surfaces: a DFT study

Ana Lucía Reviglio,* Paula S. Cappellari,* German J. Soldano,* Marcelo M. Mariscal and Gabriel A. Planes

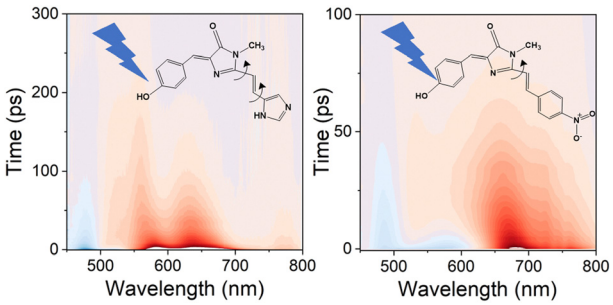
29036

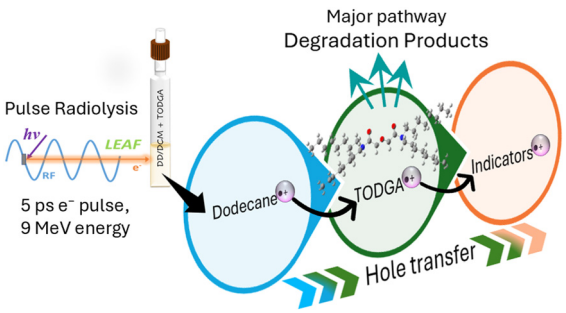


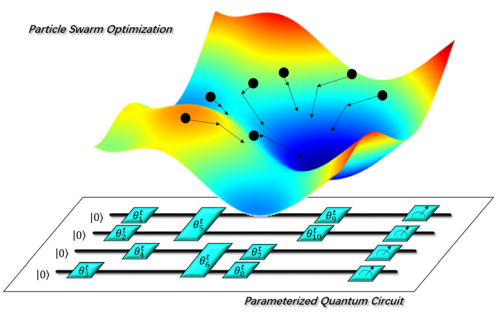
Polarization-resolved resonant Raman excitation of surface and bulk electronic bands and phonons in MBE-grown topological insulator thin films

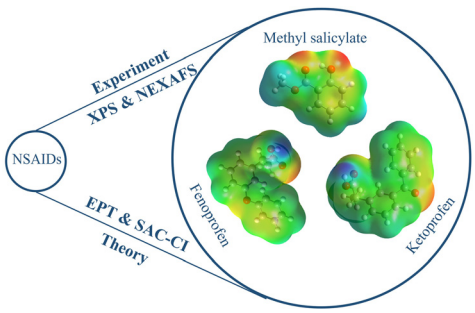
N. Kumar,* D. V. Ishchenko, I. A. Milekhin, P. A. Yunin, E. D. Kyrova, A. V. Korsakov and O. E. Tereshchenko

RESEARCH PAPERS



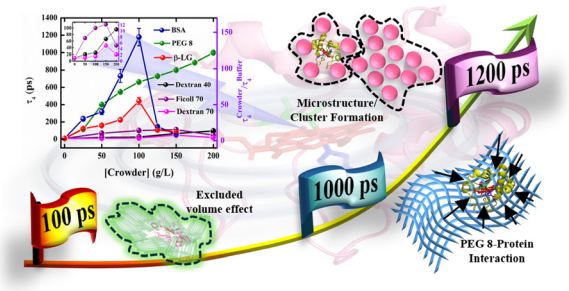






RESEARCH PAPERS

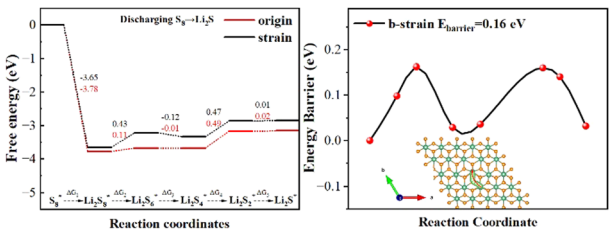
29095



Capturing ultrafast energy flow of a heme protein in crowded milieu

Shubhangi Majumdar, Ambika Prasad Kar, Jaydeep Basu and Pramit K. Chowdhury*

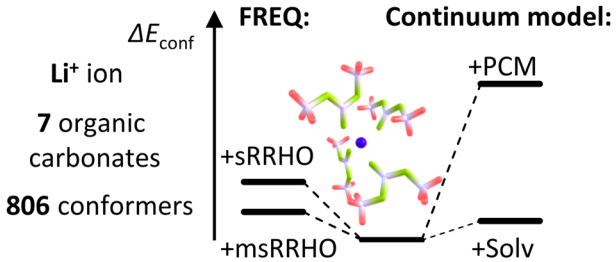
29110



Uniaxial tensile strain impact on 1T-NbS_2 monolayers as cathode material for lithium–sulfur batteries

Shanling Ren,* Xiaocong Tan, Xin Huang, Zhihong Yang and Yunhui Wang*

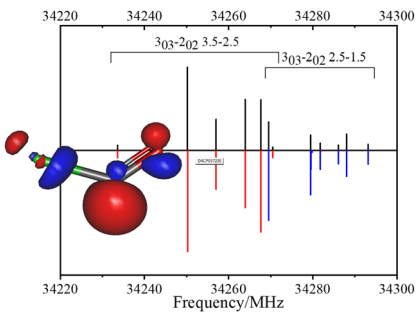
29121



A comprehensive guide for accurate conformational energies of microsolvated Li^+ clusters with organic carbonates

Arseniy A. Otlyotov, Andrey D. Moshchenkov, Timofey P. Rozov, Anna A. Tuma, Alexander S. Ryzhako and Yury Minenkov*

29133



Fourier-transform microwave spectroscopy of the ClCO radical

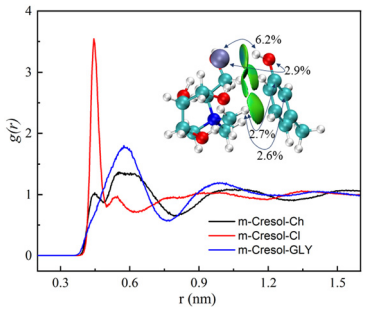
Chin-Hua Chang, Chen-Hand Tsai and Yasuki Endo*

RESEARCH PAPERS

29140

Extraction mechanism of phenolic compounds by a choline chloride/glycerol solvent: DFT and molecular dynamics studies

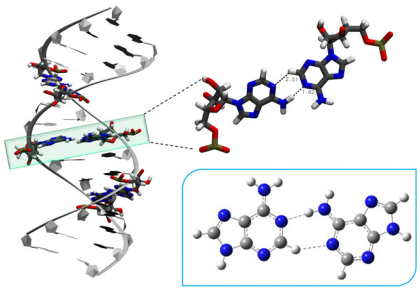
Lan Yi,* Jinwen Wang, Jixing Liu, Hao Luo, Xiaoqin Wu and Wen-Ying Li*



29150

Intermolecular hydrogen bonding delineates the stability of non-canonical adenine base pairs: a first-principles study

Nicholas Adu-Effah and Nabanita Saikia*


C-H…N and N-H…N non-canonical interaction