

IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(47) 25189–25700 (2025)



Cover

See Timothy B. Huber and Ralph A. Wheeler, pp. 25282–25291. Image reproduced by permission of Ralph A. Wheeler from *Phys. Chem. Chem. Phys.*, 2025, 27, 25282. Image partly generated with AI.



Inside cover

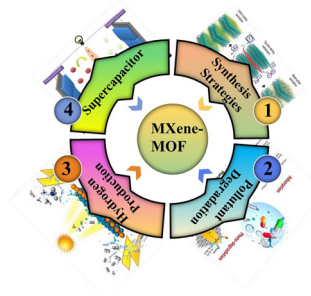
See Hui-Yan Zhao, Ying Liu *et al.*, pp. 25292–25299. Image reproduced by permission of Ying Liu from *Phys. Chem. Chem. Phys.*, 2025, 27, 25292.

REVIEWS

25204

Bridging MOFs and MXenes: from synthesis to environmental and energy technologies

Muhammad Kashif, Syed Izaz Ali Shah, Salman Khan, Sheraz Ahmad, Muhammad Anwar, Sami Ur Rahman, Shohreh Azizi* and Malik Maaza



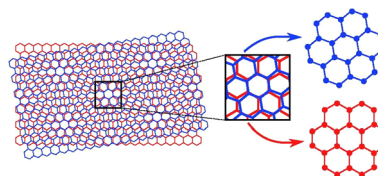
25232

Review of the tight-binding method applicable to the properties of moiré superlattices

Xueheng Kuang, Federico Escudero, Pierre A. Pantaleón, Francisco Guinea and Zhen Zhan*

Tight-binding model

$$H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{\langle i,j \rangle} t_{ij} c_i^\dagger c_j$$



Royal Society of Chemistry approved training courses

Explore your options.
Develop your skills.
Discover learning
that suits you.

**Courses in the classroom,
the lab, or online**

Find something for every
stage of your professional
development. Search our
database by:

- subject area
- location
- event type
- skill level

Members **get at least 10% off**

Visit rsc.li/cpd-training



**SAVE
10%**

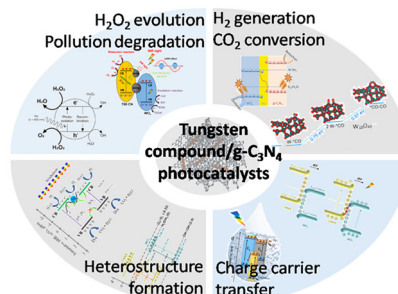


TUTORIAL REVIEW

25254

Enhanced charge carrier separation and transfer in g-C₃N₄ and tungsten oxide/sulfide composite photocatalysts

Xiao Zhang* and Ping Yang*

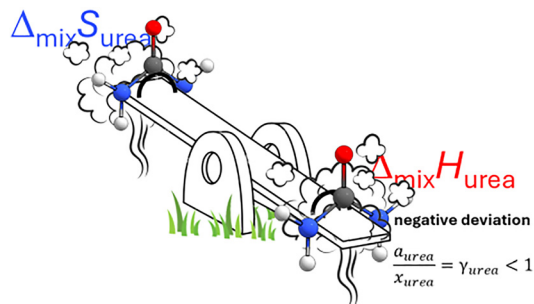


COMMUNICATIONS

25266

Direct experimental verification of negative deviations from ideal mixing in an archetypal deep eutectic solvent

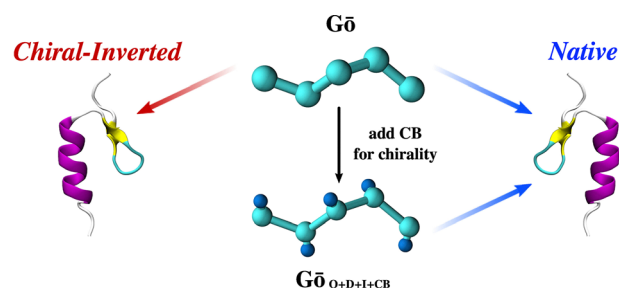
Francesco I. Travaglini, Lorenza Romagnoli,*
 Angelika M. Czerska, Matteo Busato, Giorgia Mannucci,
 Stefano Vecchio Cipriotti, Paola D'Angelo and
 Andrea Ciccioni*



25271

Key parameters for accurate chiral folding and mechanics in G \bar{o} -like coarse-grained potentials

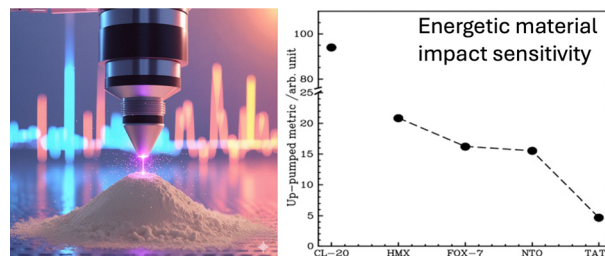
Yi-Chen Tsai and Chi-cheng Chiu*



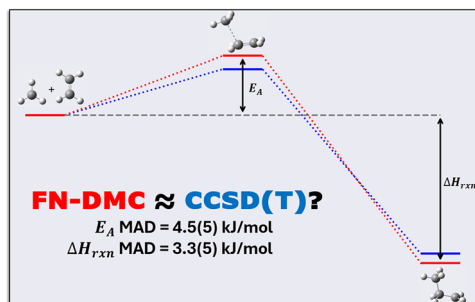
25276

Evaluating the impact sensitivity of energetic materials using inelastic neutron scattering and low frequency THz-Raman spectroscopies

Adam A. L. Michalchuk,* Carole A. Morrison,*
 Colin R. Pulham and Svemir Rudić



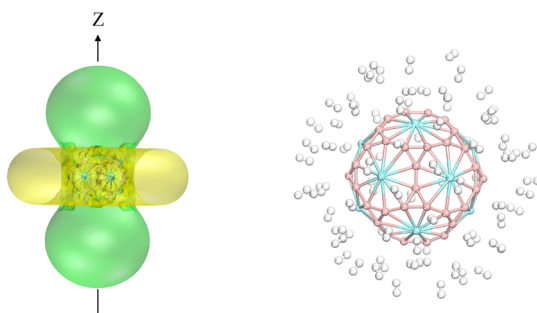
25282



Fixed node-diffusion Monte Carlo achieves chemical accuracy in predicting substituent effects on activation energies and reaction enthalpies for methyl radical addition to substituted olefins

Timothy B. Huber* and Ralph A. Wheeler*

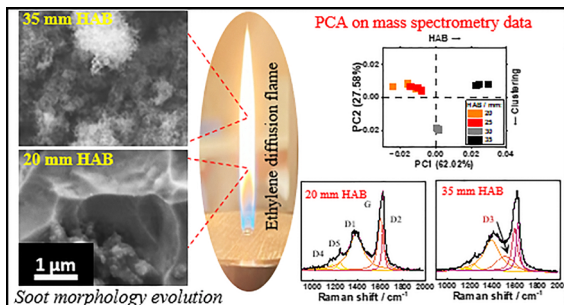
25292



Aromatic $M_{12}B_{60}$ ($M = Y, Lu$) metallo-borospherenes for reversible hydrogen storage

Yi-Sha Chen, Jing-Jing Guo, Peng-Bo Liu, Hui-Yan Zhao,* Jing Wang and Ying Liu*

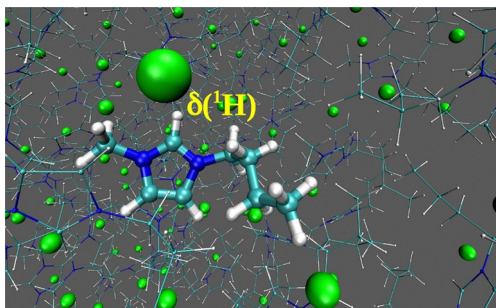
25300



Ex situ characterization of the precursors of incipient nanoparticles in a laminar diffusion flame of ethylene

Harsh Chaliyawala, Erin McCaughey, Xavier Mercier, J. Houston Miller, Myriam Moreau, Nicolas Nuns, Pardis Simon and Alessandro Faccineto*

25310



Towards quantitative prediction of proton chemical shifts in imidazolium chloride ionic liquids by computational NMR

Ruijian Zhu, Tianying Yan, Yanting Wang* and Giacomo Saielli*

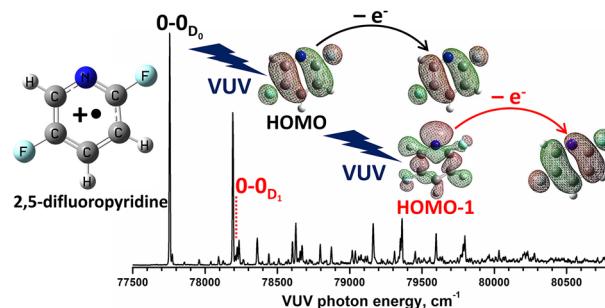


RESEARCH PAPERS

25322

Resolving ionization-induced distortions in 2,5-difluoropyridine: influences of *meta*-fluorination on electronic and vibrational structures

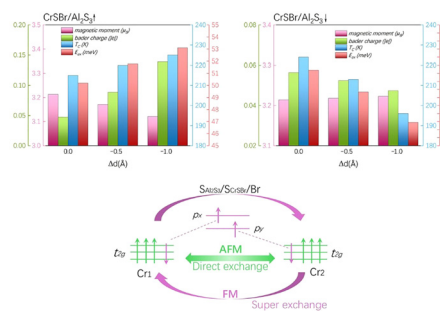
Hyojung Kim, Sung Man Park and Chan Ho Kwon*



25330

Nonvolatile electric control of magnetic anisotropy and Curie temperature in the van der Waals multiferroic heterostructure CrSBr/Al₂S₃

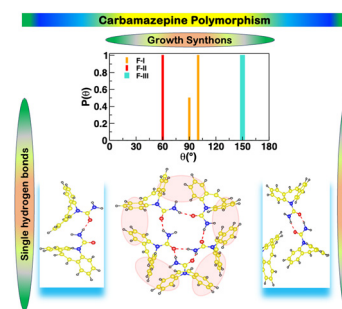
Xiaotong Zhou and Baozeng Zhou*



25342

Molecular dynamics simulations on the effect of solvent and supersaturation on the aggregation behaviour in carbamazepine

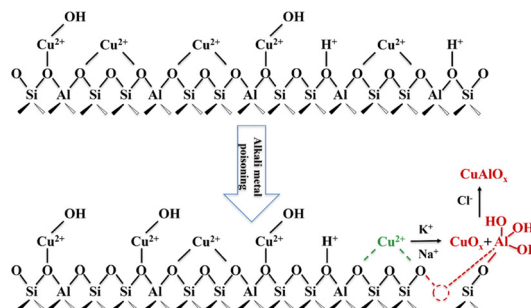
Manju Sharma* and Shampita Saha



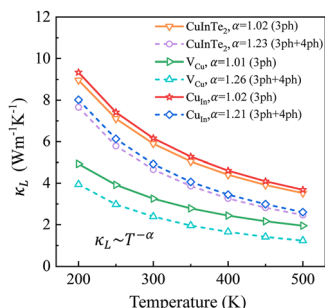
25352

Effect of alkali metal poisoning on Cu-SSZ-13 in selective catalytic reduction with ammonia (NH₃-SCR)

Boji Wang, Yao Zhang, Sarayute Chansai, Junling Zhan, Huaizhong Xiang, Tengfei He, Yilai Jiao, Yu Zhang* and Xiaolei Fan*



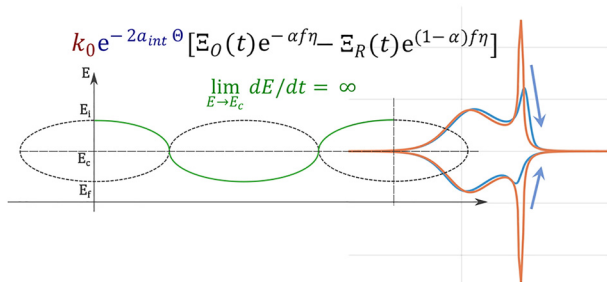
25365



Unveiling the impact of intrinsic defects on thermal conductivity in CuInTe₂ using neural network potential

Wenjin Li, Yongwei Tang, Qingbo Liu, Ziyang Yu,*
Shiheng Liang, Zhihong Lu, Rui Xiong and Pan Zhang*

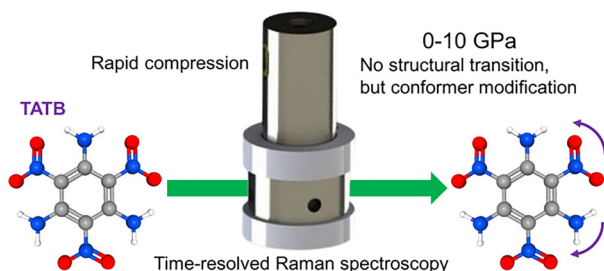
25374



Asymmetries in elliptic cyclic voltammograms of strongly-adsorbed redox couples: kinetics or thermodynamics?

Manuel Antuch

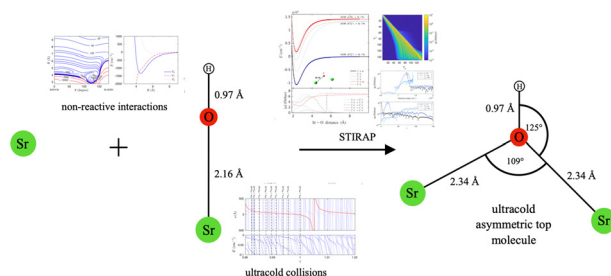
25383



High pressure structural properties of 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) under rapid compression

XiaoHui Chen, Yi Zhang, Yuncan Ma, Lei Liu, Shijia Ye,
Shourui Li, Qiumin Jing, Junjie Gao, Hao Wang,
Chuanlong Lin, Jun Li* and Qiang Wu*

25389



Production of ultracold asymmetric tops from Sr atoms and SrOH molecules

Maciej B. Kosicki,* Mateusz Borkowski, Marcin Umiński
and Piotr S. Żuchowski

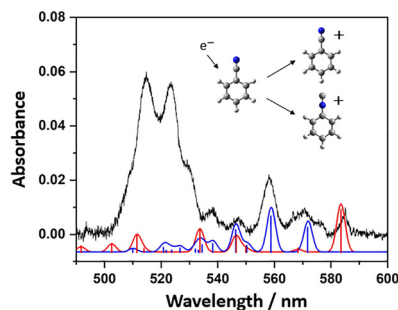


RESEARCH PAPERS

25405

Visible absorption spectra of mass-selected cyanobenzene and iso-cyanobenzene cations in solid neon

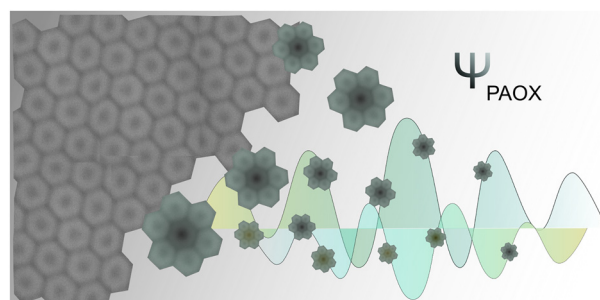
Shu-Yu Lin, Sheng-Lung Chou, Wen-Jian Huang, Chih-Hao Chin, Chien-Ming Tseng* and Yu-Jong Wu*



25412

Quantum mechanical aspects of order evolution processes – the case of nanoporous aluminum oxide

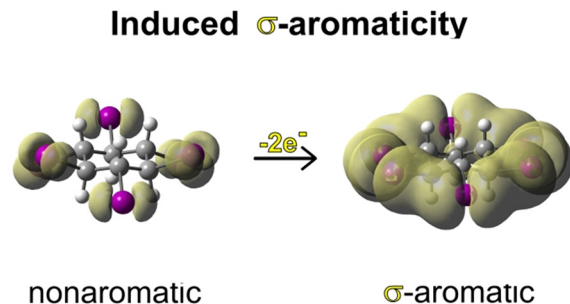
Silvio Heinschke* and Jörg J. Schneider



25422

Oxidation-induced σ -aromaticity in halogenated cycloalkanes

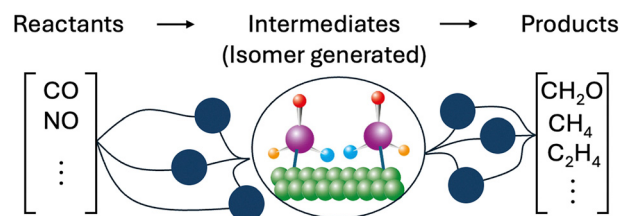
Slavko Radenković* and Slađana Đorđević



25433

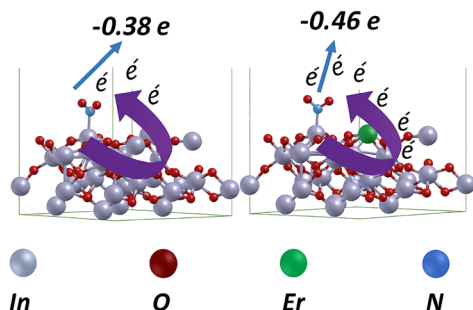
Atomistic catalytic reaction networks: case study on electrochemical reduction of CO, NO & combinations

Alexander Bagger* and Amy Wuttke



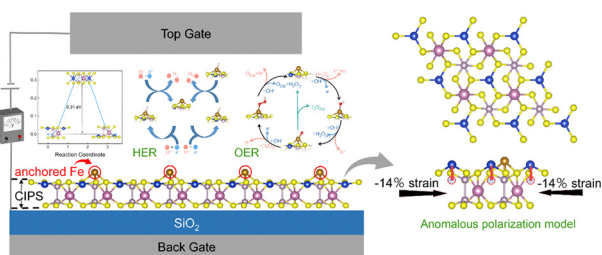
RESEARCH PAPERS

25440

Effect of Er doping on the $\text{In}_2\text{O}_3(001)$ surface for H_2S , NO_2 , and CO detection: a DFT study

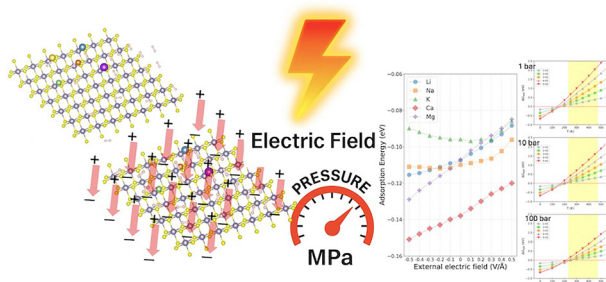
Neha Sharma and Sandip Paul Choudhury*

25449

Deciphering the regulatory mechanism of electrocatalytic activity in an Fe-anchored CuInP_2S_6 monolayer via ferroelectric switching and in-plane strain

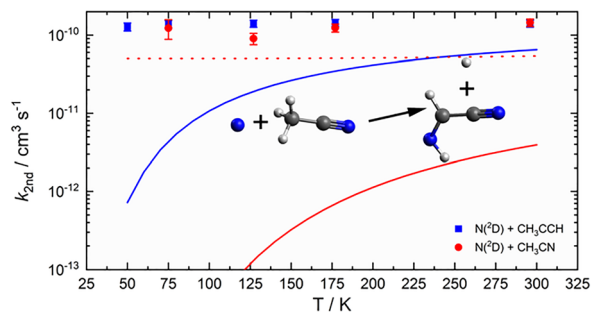
Wenjing Jiang, Jiahui Tang, Dazhi Sun* and Baozeng Zhou*

25462

Enhancing hydrogen adsorption on SnS_2 and SnSe_2 monolayers: alkali and alkaline earth metal decoration under external electric fields

Audomsak Sriphothongnack, Watcharin Teeranattapong, Supparat Charoenphon, Adisak Boonchun, Thanayut Kaewmaraya and Pakpoom Reunchan*

25474

A gas-phase kinetic study of the $\text{N}(^2\text{D}) + \text{CH}_3\text{CCH}$ and $\text{N}(^2\text{D}) + \text{CH}_3\text{CN}$ reactions

Kevin M. Hickson,* Jean-Christophe Loison, Benjamin Benne and Michel Dobrijevic

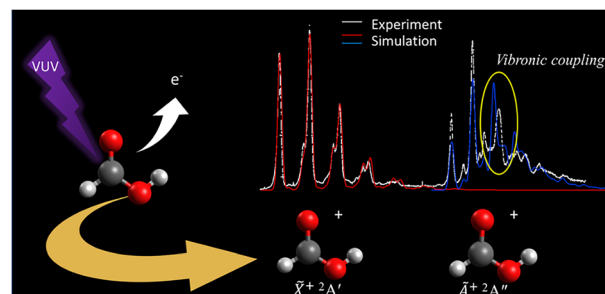


RESEARCH PAPERS

25483

A study on the spectroscopy of *cis*- and *trans*-formic acid upon ionisation

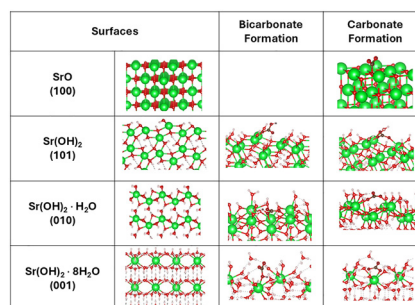
A. Gloriod, M. Mogren Al-Mogren and M. Hochlaf*



25498

Understanding CO₂ adsorption on the surfaces of SrO and its hydroxylated variants Sr(OH)₂·nH₂O (n = 0, 1, 8)

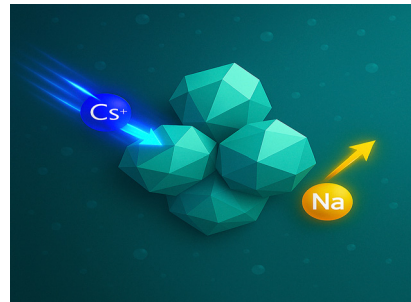
Manh Tien Nguyen, Dominic R. Alfonso, Douglas R. Kauffman, Chris M. Marin, Qing Shao and Yuhua Duan*



25512

Energetics and kinetics of alkali ion exchange in analcime

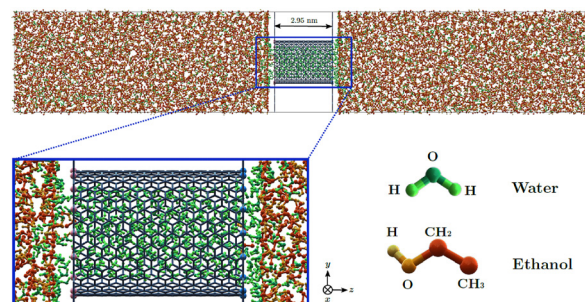
Jinyi Liu, An T. Ta, R. Seaton Ullberg, Jean Wilfried Hounfodji, Michael Badawi, Hans-Conrad zur Loye and Simon R. Phillpot*



25524

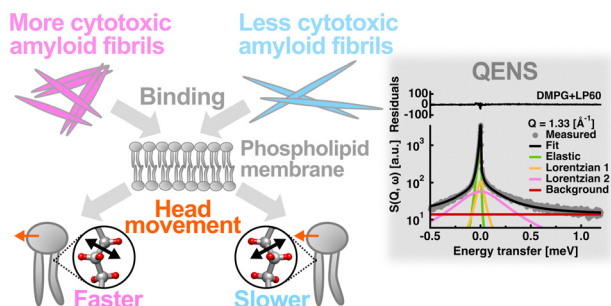
Water–ethanol separation with Janus tip charged carbon nanotubes

Yûi Ono, Eiji Yamamoto and Kenji Yasuoka*



RESEARCH PAPERS

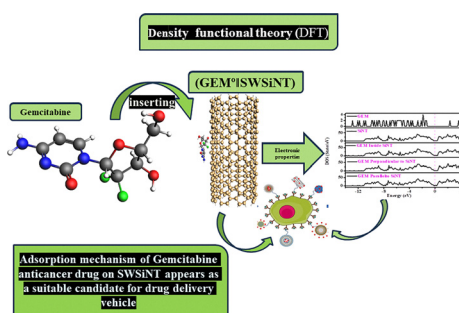
25536



Dynamical changes of phospholipid membranes caused by polymorphic amyloid fibrils studied by quasi-elastic neutron scattering

Tatsuhito Matsuo,* Seigi Yamamoto, Taiki Tominaga and Judith Peters*

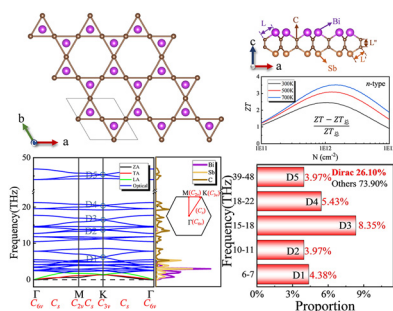
25547



Exploring the adsorption of Gemcitabine on silicon nanotubes using density functional theory

Saleh S. Alarfaji, Ume Kalsoom, Rabia Gilani and Muhammad Isa Khan*

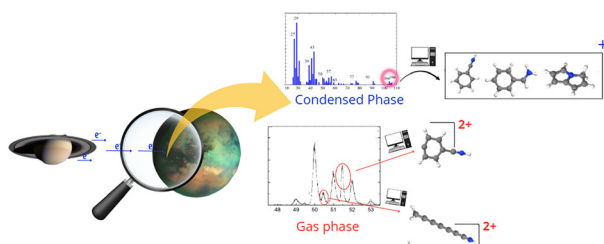
25558



First-principles study of the effect of multi-Dirac phonons on the thermoelectric properties of the Janus BiSbC_3 monolayer

Hui-Xue Shen, Xiao-Wen Wang, Qing Lu,*
Xiao-Lin Zhou, Yi Mu and Cai Cheng*

25569



Condensed and gaseous benzonitrile: ionic species formation and structural parameters

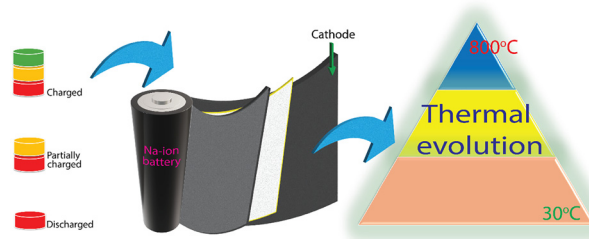
Jorge H. C. Basilio, Ricardo R. Oliveira,*
Roberto Nascimento, Maria Luiza M. Rocco,
Lucia H. Coutinho, Fabio de A. Ribeiro and Wania Wolff*



25581

Thermal evolution of cathode materials used in commercial sodium-ion batteries

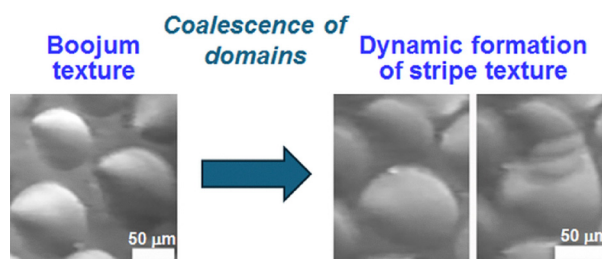
B. D. K. K. Thilakarathna, Timothy A. Ablott, Taren Cataldo, Pria Ramkissoon, Govardhan Sontam and Neeraj Sharma*



25593

Liquid condensed domain coalescence-induced modulated structure formation in Langmuir monolayers: monolayer meets topology via elasticity and geometry

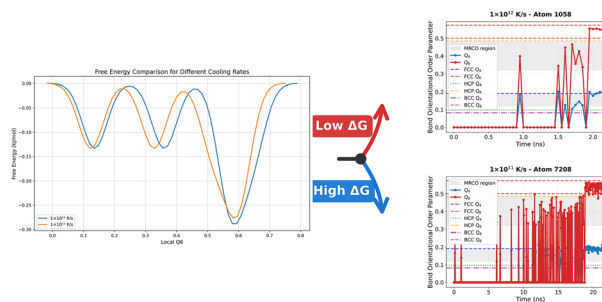
E. Hatta



25604

Effect of cooling rate on the formation pathway of medium-range FCC nanocrystals: the role of MRCO in structural evolution

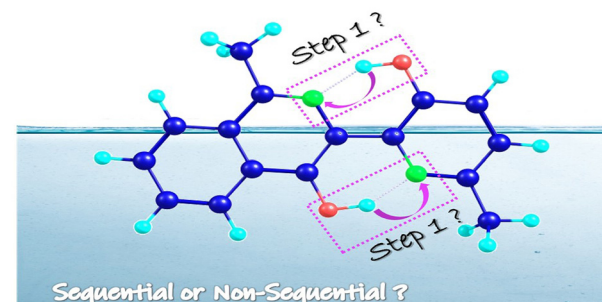
Zhi-Hao Zhao



25613

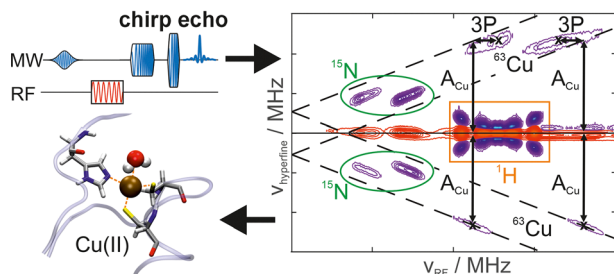
Computational unveiling of solvent-polarity-dependent ESDPT behavior in typical asymmetric PIQ fluorophores

Zibo Shen, Chang Liu, Jinfeng Zhao* and Jiahe Chen*



25624

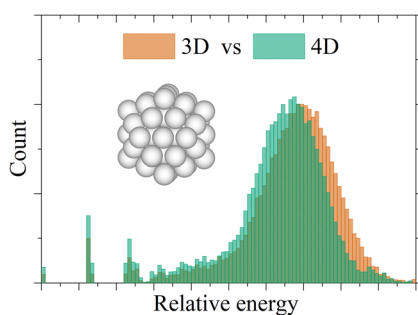
CHEESY ENDOR



Resolving spectral overlap in ENDOR by chirp echo Fourier transform detection

Julian Stropp, Fabia Canonica, Nino Wili* and Daniel Klose*

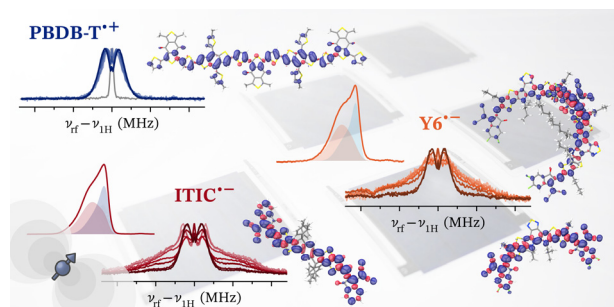
25636



Improving structure search with hyperspatial optimization and TETRIS seeding

Daviti Gochitashvili, Maxwell Meyers, Cindy Wang and Aleksey N. Kolmogorov*

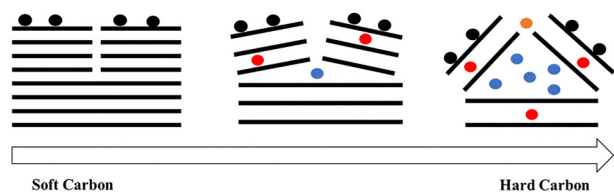
25648



Charge and spin delocalisation in photoinduced polarons of polymer donors and non-fullerene acceptors for organic photovoltaics – a multi-frequency pulse EPR study

Jack M. S. Palmer, Oliver Christie and Claudia E. Tait*

25663



The change of Na storage mechanism from soft carbon to hard carbon

Huy Sy Nguyen* and Arnulf Latz

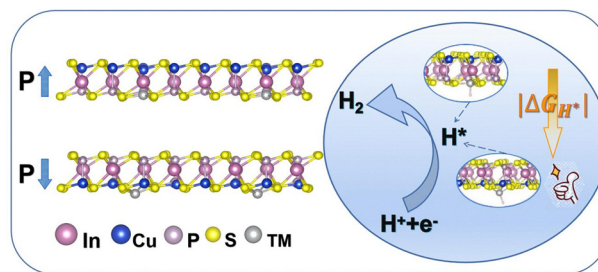


RESEARCH PAPERS

25675

Tunable hydrogen production of a transition metal-anchored CuInP_2S_6 monolayer with a ferroelectric switch

Shiqi Huang, Tingting Bo, Nan Mu, Shiyu Liu, Wei Zhou,*
Dejun Li* and Yanyu Liu*



25684

Unveiling the role of the amino nitrogen–ruthenium cooperation effect in methanol steam reforming reaction *via* hydride transfer mechanism and Marcus theory

Koushik Makhal and Bhabani S. Mallik*

