

PCCP

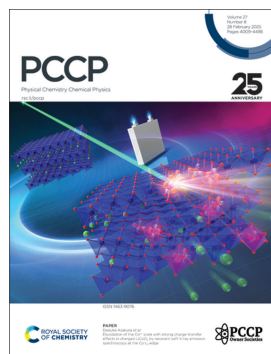
Physical Chemistry Chemical Physics – An international journal

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 27(8) 4009–4498 (2025)



Cover

See Daisuke Asakura *et al.*, pp. 4092–4098. Image reproduced by permission of National Institute of Advanced Industrial Science and Technology from *Phys. Chem. Chem. Phys.*, 2025, 27, 4092.



Inside cover

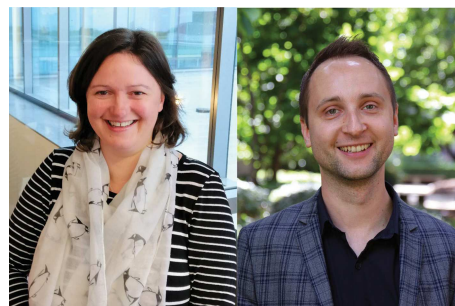
See Célia Fonseca Guerra *et al.*, pp. 4099–4108. Image reproduced by permission of Celine Nieuwland and Célia Fonseca Guerra from *Phys. Chem. Chem. Phys.*, 2025, 27, 4099.

EDITORIAL

4023

Showcasing physical chemistry research in Australia and New Zealand – a vital nexus of innovation and opportunity

Sarah L. Masters* and Lars Goerigk*

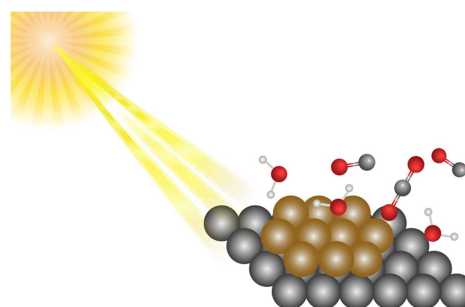


PERSPECTIVE

4025

The need for robust model systems in the study of hybrid interfaces for photocatalysis and photoelectrocatalysis

Mekha P. Mohandas and Jared P. Bruce*



EES Catalysis

GOLD
OPEN
ACCESS

Exceptional research on energy and environmental catalysis

Open to everyone. Impactful for all

rsc.li/EESCatalysis

Fundamental questions
Elemental answers

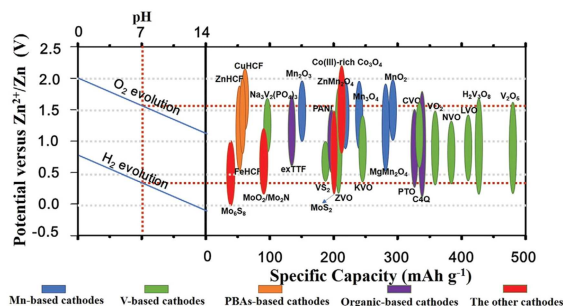


REVIEW

4045

Non-rechargeable batteries: a review of primary battery technology and future trends

Jahanvi Thakur, Peeyush Phogat,* Shreya, Ranjana Jha and Sukhvir Singh

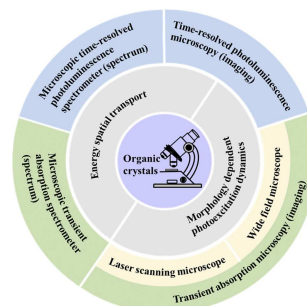


TUTORIAL REVIEW

4078

Microscopic time-resolved spectroscopy of organic crystals at the nanometer and micrometer scale

Xi Liu, Minjie Li and Yan Wan*

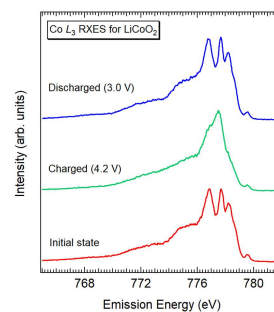


RESEARCH PAPERS

4092

Elucidation of the Co⁴⁺ state with strong charge-transfer effects in charged LiCoO₂ by resonant soft X-ray emission spectroscopy at the Co L₃ edge

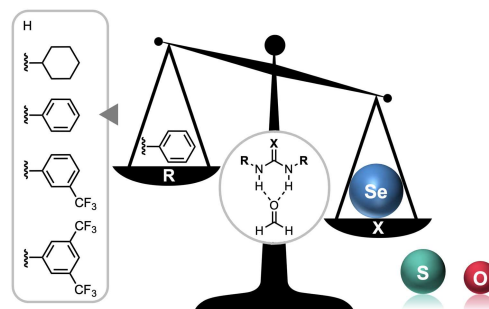
Daisuke Asakura,* Takaaki Sudayama, Yusuke Nanba, Eiji Hosono, Hisao Kiuchi, Kosuke Yamazoe, Jun Miyawaki, Yoshihisa Harada, Atsuo Yamada, Ru-Pan Wang and Frank M. F. de Groot



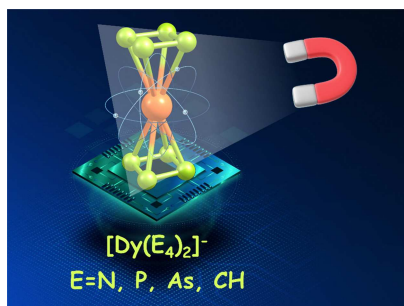
4099

Urea hydrogen-bond donor strengths: bigger is not always better

Celine Nieuwland, Angelina N. van Dam, F. Matthias Bickelhaupt and Célia Fonseca Guerra*



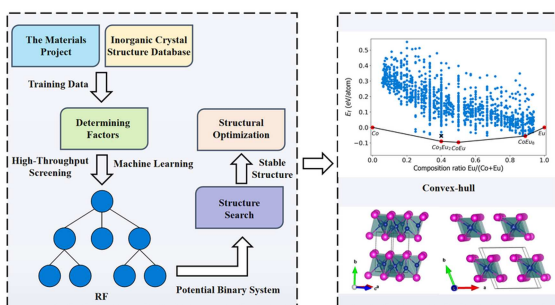
4109



Unravelling the electronic structure, bonding, and magnetic properties of inorganic dysprosocene analogues [Dy(E₄)₂]⁻ (E = N, P, As, CH)

Ibtesham Tarannum and Saurabh Kumar Singh*

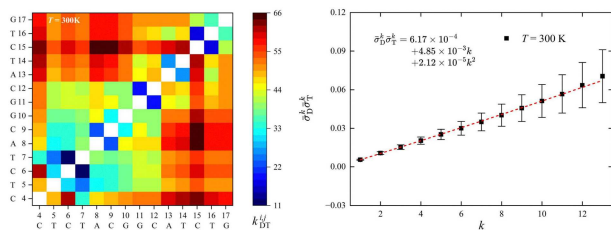
4121



Predicting miscibility in binary compounds: a machine learning and genetic algorithm study

Chiwen Feng, Yanwei Liang, Jiaying Sun, Renhai Wang,*
Huajun Sun* and Huafeng Dong

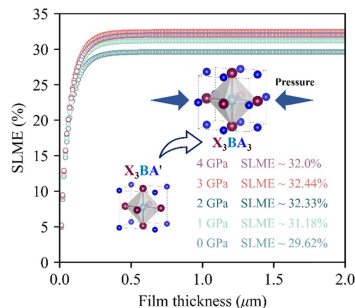
4129



Temperature-induced swelling and unwinding of double-stranded DNA

Tingting Liu, Kai Liu, Xuankang Mou and Shibei Li*

4144



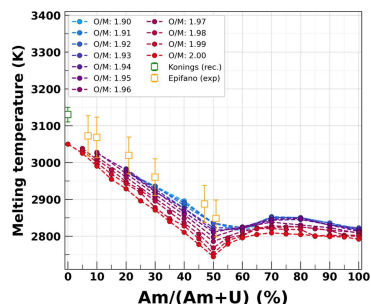
Pressure-dependent optoelectronic properties of antiperovskite derivatives X₃AsCl₃ (X = Mg, Ca, Sr, Ba): a first-principles study

Tao Hu, Changhe Wu, Mingjun Li, Hao Qu, Xin Luo,
Yihao Hou, Shichang Li, Shengnan Duan, Dengfeng Li,*
Gang Tang* and Chunbao Feng*

4152

Systematic study of the structural, energetic and elastic properties of $U_{1-y}Am_yO_{2-x}$ compounds using empirical interatomic potentials

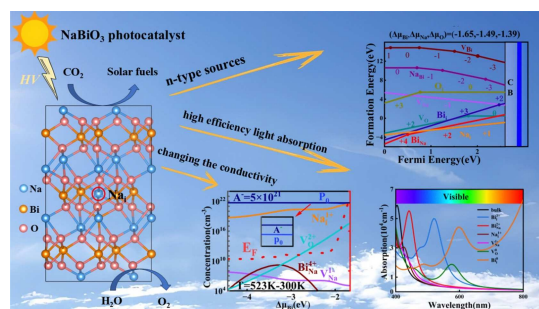
Baptiste Labonne, Christine Guéneau and Marjorie Bertolus*



4172

Defect physics investigations in bulk $NaBiO_3$ photocatalysts via Heyd–Scuseria–Ernzerhof hybrid density functional theory calculations

Song Ling, Jingcheng Wang, Bo Kong,* Ti-xian Zeng* and Wentao Wang*

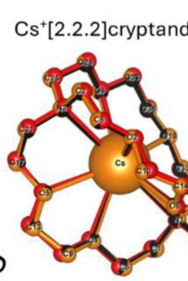


4187

Prediction of NMR parameters and geometry in ^{133}Cs -containing compounds using density functional theory

N. Manukovsky, N. Vaisleib, M. Arbel-Haddad and A. Goldbourt*

Experimental
 $V=1235 \text{ \AA}^3$
 $\delta_{iso}=225 \text{ ppm}$
 $Cq=1047 \text{ kHz}$



PBE
 $V=1438 \text{ \AA}^3$
 $\delta_{iso}=254.3 \text{ ppm}$
 $Cq=959 \text{ kHz}$

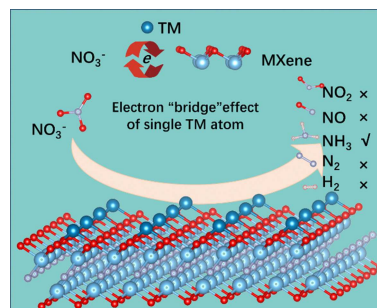
^{133}Cs DFT/NMR

rev-vdW-DF2
 $V=1209 \text{ \AA}^3$
 $\delta_{iso}=228.7 \text{ ppm}$
 $Cq=1071 \text{ kHz}$

4202

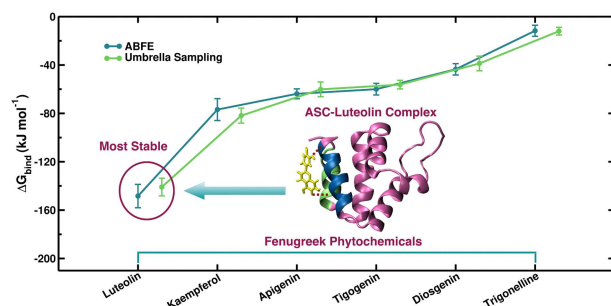
Revealing the origin of activity and selectivity in nitrate to ammonia conversion on single transition metal atom catalysts supported by a Ti_2NO_2 monolayer

Yuwen Cheng,* Wenjie Wang and Cuiping Shao



RESEARCH PAPERS

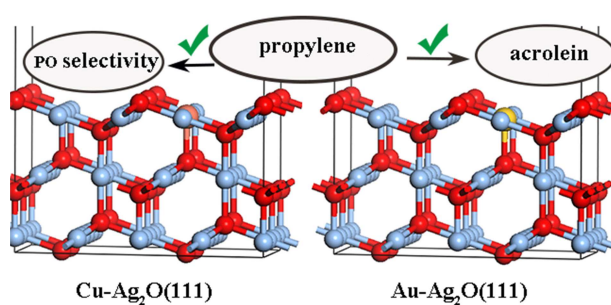
4211



Thermodynamic origin of fenugreek phytochemical binding to the ASC pyrin domain for inflammation inhibition

Avinash Garg and Ananya Debnath*

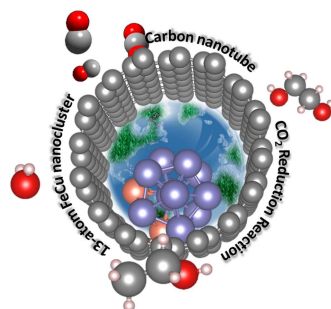
4222



Effect of Cu/Au for propylene epoxidation over the $\text{Ag}_2\text{O}(111)$ surface: a DFT study

Zean Xie, Xin Wang, Simeng Zhao, Ke Zhang, Yangyang Song,* Guichang Wang* and Zhen Zhao*

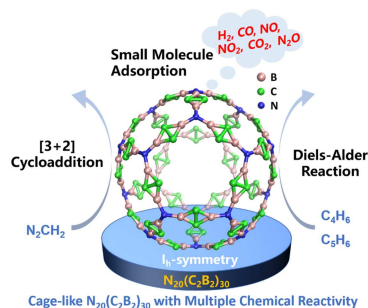
4234



The roles of various Fe–Cu bimetallic nanoclusters in controlling the C2 selectivity for the CO reduction reaction – a DFT study

Chen-Cheng Liao, Meng-Chi Hsieh, Yung-Yi Huang, Cheng-Yu Tu and Chun-Chih Chang*

4246



High-symmetry cage-like molecule $\text{N}_{20}(\text{C}_2\text{B}_2)_{30}$: computational insight into its bonding and reactivity

Miaorun Zhang, Lin Zhang, Zexing Cao and Yi Zhao*

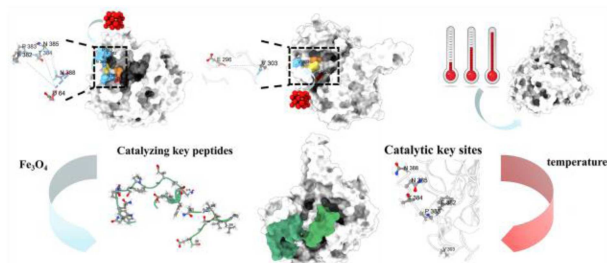


RESEARCH PAPERS

4253

The effect of the allosteric regulation on the catalytic activity of fructosyltransferase studied via molecular dynamics simulations

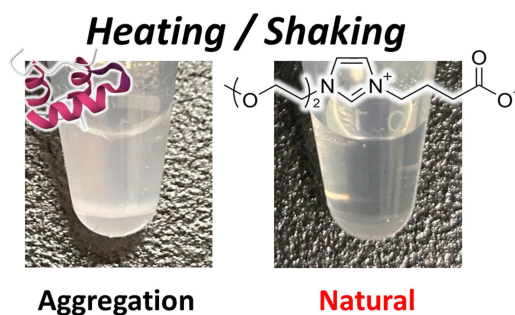
Chaofan Yu, Yanqi Liu, Liang Fu, Zhengyu Shu, Mojie Duan* and Yi Zheng*



4263

Stabilizing protein pharmaceuticals by imidazolium-type zwitterions

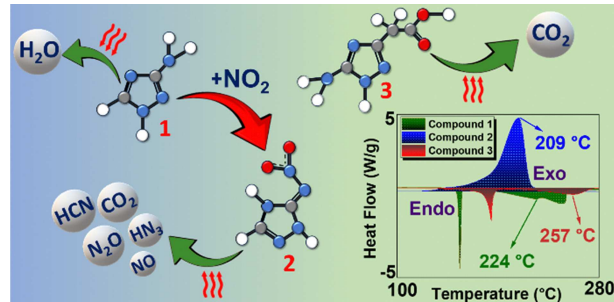
Ai Tajiri, Takeru Ishizaki, Takahiro Takekiyo, Kazuaki Ninomiya, Kenji Takahashi and Kosuke Kuroda*



4269

Insights into triazole-based energetic material design from decomposition pathways of triazole derivatives

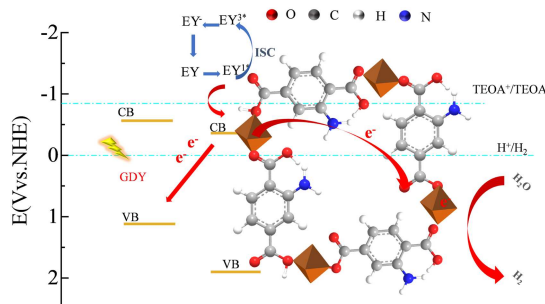
Sarika Venugopal, Shani Saha, Neeraj Kumbhakarna and Anuj A. Vargeese*



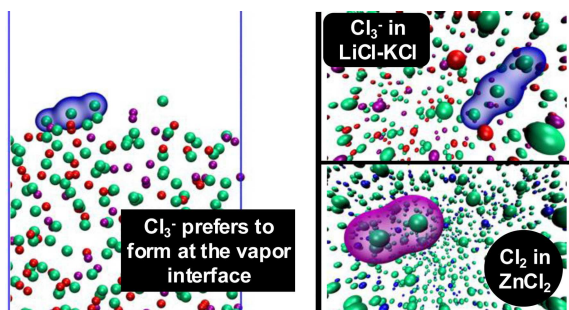
4278

Efficient photocatalytic hydrogen production by employing a graphdiyne/NH₂-MIL-88B(Fe) composite

Ziyu Li, Mei Li,* Rongsheng Xu and Zhiliang Jin



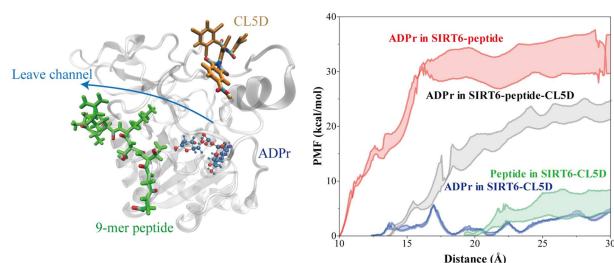
4290



Chlorine gas and anion radical reactivity in molten salts and the link to chlorobasicity

Hung H. Nguyen, Luke D. Gibson, Matthew S. Emerson, Bichitra Borah, Santanu Roy,* Vyacheslav S. Bryantsev* and Claudio J. Margulis*

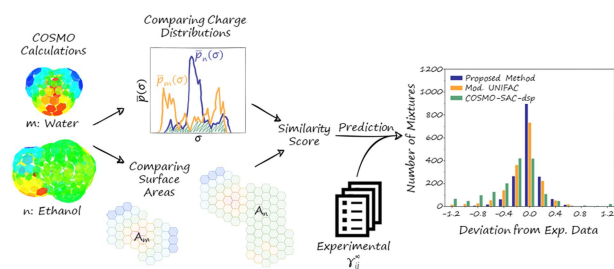
4298



Molecular dynamics simulation on the role of CL5D in accelerating the product dissociation of SIRT6

Hao Rao, Ting Yang, Yue Wang, Junwen Fei, Li-Hua Bie* and Jun Gao*

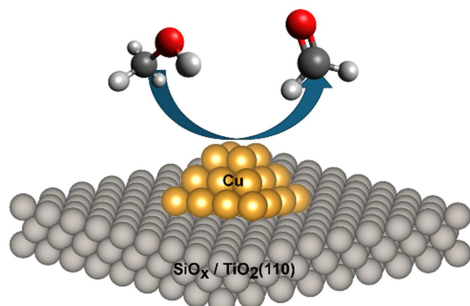
4307



Prediction of activity coefficients by similarity-based imputation using quantum-chemical descriptors

Nicolas Hayer, Thomas Specht, Justus Arweiler, Dominik Gond, Hans Hasse and Fabian Jirasek*

4316



Conversion of methanol at copper clusters on TiO₂(110) and SiO_x: direct dehydrogenation vs. partial oxidation and influence of cluster size and substrate

Maximilian Grebien and Katharina Al-Shamery*

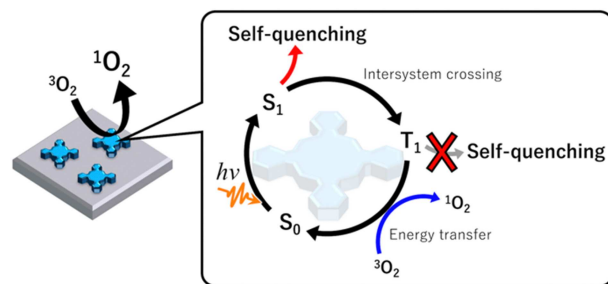


RESEARCH PAPERS

4328

Effect of excited state self-quenching on singlet oxygen photogeneration using nanosheet surface assembled zinc phthalocyanine

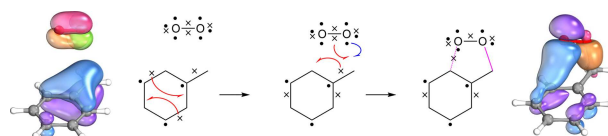
Takuya Fujimura,* Kazuya Okada, Masatoshi Nishiguchi, Yasuyuki Araki, Takahisa Ikeue and Ryo Sasai*



4335

Benzylperoxy radical cation: an exceptionally stable and bound species

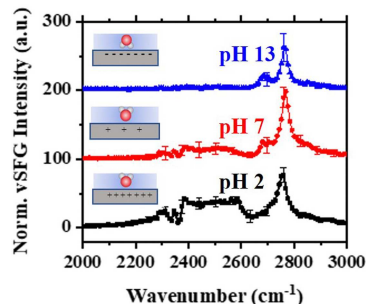
Chow-Shing Lam, Xi-Guang Wei, Yi Pan and Kai-Chung Lau*



4343

pH-dependent reactivity of water at MgO(100) and MgO(111) surfaces

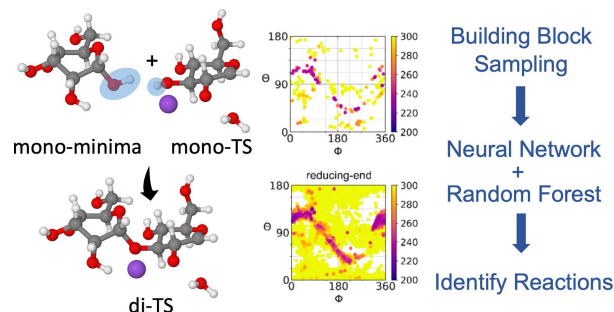
Narendra M. Adhikari,* Piotr Zarzycki, Zheming Wang and Kevin M. Rosso*



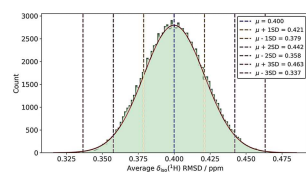
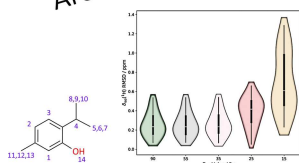
4355

Using building block structures and a cooperative approach with neural networks and random forest to identify reactions: a case study on the dissociation of sodiated disaccharides

Pei-Kang Tsou, Huu Trong Phan and Jer-Lai Kuo*

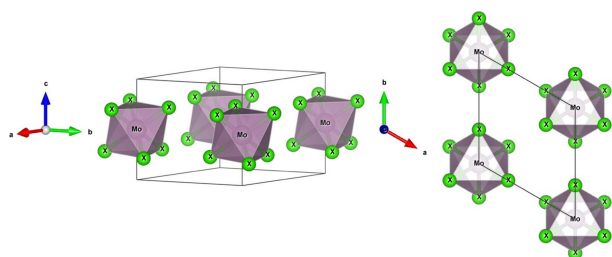


4368

Thymol, Where
Are You????More Efficient
GIPAW DFT ¹H Shifts**¹H isotropic chemical shift metrics for NMR crystallography of powdered molecular organics**

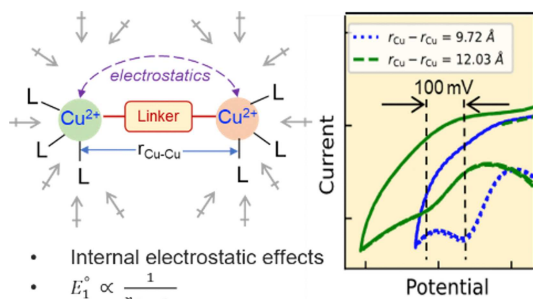
Fatemeh Zakeri and Cory M. Widdifield*

4383

**Exploring the physical properties of the new MoX₆ (X = Cl or Br) materials**

A. Jabar, N. Maaouni, S. Benyoussef and L. Bahmad*

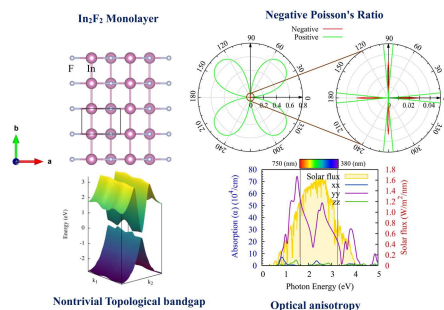
4398

**Influence of internal electrostatics on reduction potentials in amine-ligated bimetallic copper complexes**

Prateek Saini, Shubham Gupta and Srinivasan Ramakrishnan*

- Internal electrostatic effects
- $E_1^0 \propto \frac{1}{r_{Cu-Cu}}$

4407

**In₂F₂ monolayer: a new class of two-dimensional materials with negative Poisson's ratio and topological phase**

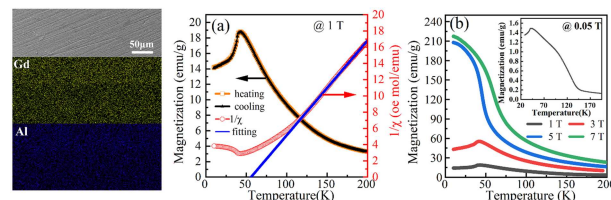
Shahram Yalameha,* Javad Zahmatkesh, Fatemeh Zamanian and Zahra Nourbakhsh



4419

First-order non-hysteretic phase transition: a pathway to enhanced magnetocaloric and giant magnetoresistance effects in a Gd–Al alloy

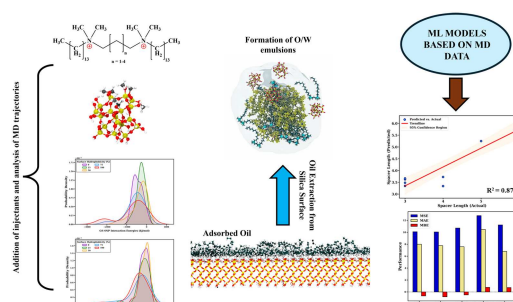
Guiquan Yao, Peng Gao, Zonghang Liu,* Che Zhang,* Guangzhao Wang and Weibin Cui*



4429

Optimizing oil detachment from silica surfaces using gemini surfactants and functionalized silica nanoparticles: a combined molecular dynamics and machine learning approach

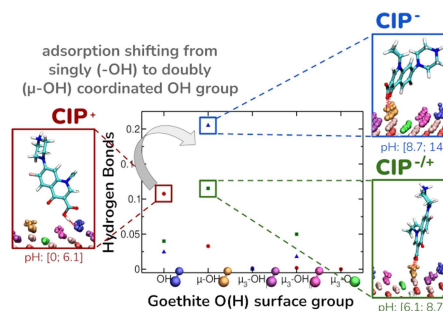
Gourav Chakraborty, Keka Ojha, Ajay Mandal and Niladri Patra*



4446

Molecular-level insight into ciprofloxacin adsorption on goethite: I. Approach and non-specific binding

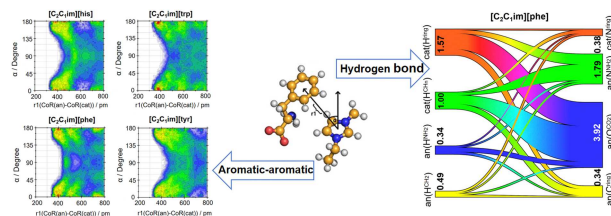
Sébastien Le Crom* and Jean-François Boily*



4457

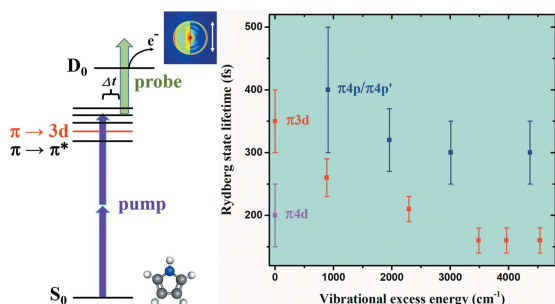
Aromatic–aromatic interactions and hydrogen bonding in amino acid based ionic liquids

Wenbo Dong, Patrick R. Batista, Jan Blasius and Barbara Kirchner*



RESEARCH PAPERS

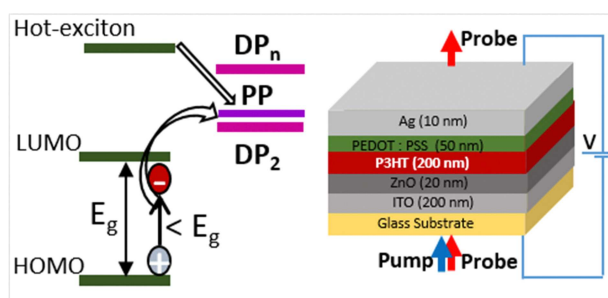
4467



Time-resolved measurements of subpicosecond excited-state lifetimes of high-lying Rydberg states in pyrrole

Dongyuan Yang,* Yuhuan Tian, Yanjun Min, Zhigang He, Guorong Wu* and Xueming Yang

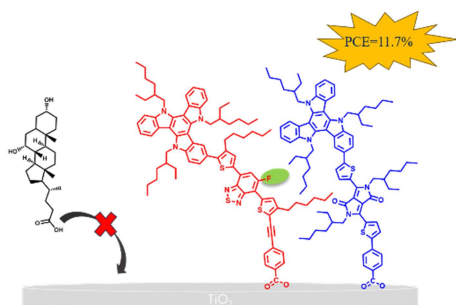
4475



Direct route of ultrafast charge-pair generation upon below-band-gap excitation in P3HT: effect of external electric field

Debkumar Rana,* Ayush Kant Ranga and Arnulf Materny*

4487



Impact of fluorine-induced effects on co-sensitization systems in dye-sensitized solar cells

Miao Jiang, Rui Wang, Gongchen Xu, Qing Shangguan, Haoxin Wang, Ming Cheng, Shiguo Sun, Li Zhang* and Xichuan Yang*

CORRECTION

4495

Correction: Symmetry-breaking charge transfer and intersystem crossing in copper phthalocyanine thin films

Esther del Pino Rosendo, Okan Yildiz, Wojciech Pisula, Tomasz Marszalek, Paul W. M. Blom and Charusheela Ramanan*

