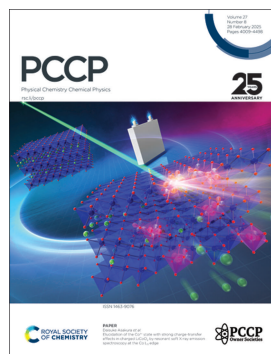


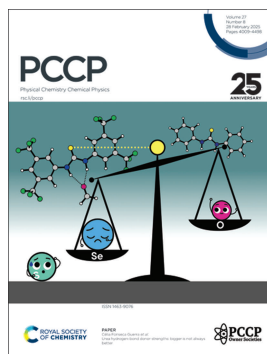
IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 27(8) 4009–4498 (2025)



Cover

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Inside cover

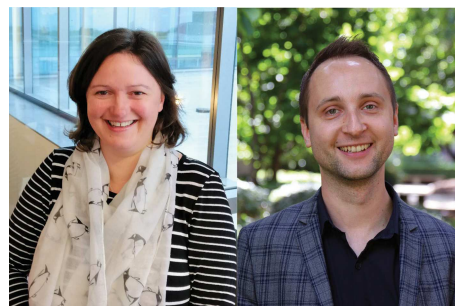
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EDITORIAL

4023

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

Sarah L. Masters* and Lars Goerigk*

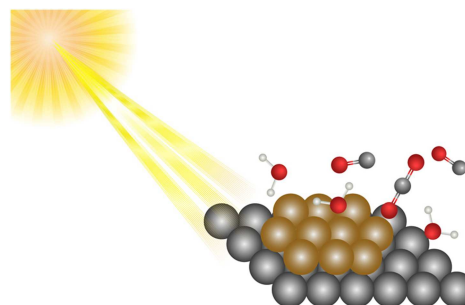


PERSPECTIVE

4025

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

Mekha P. Mohandas and Jared P. Bruce*



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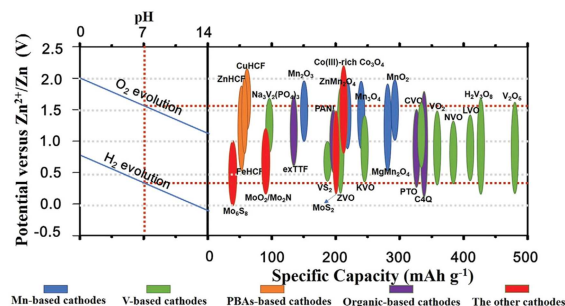
Fundamental questions
Elemental answers

REVIEW

4045

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

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

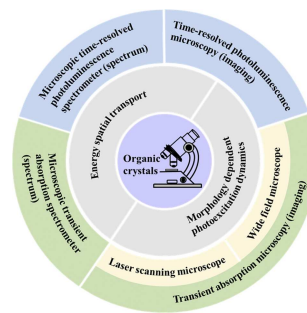


TUTORIAL REVIEW

4078

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

Xi Liu, Minjie Li and Yan Wan*

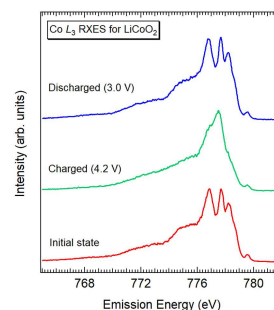


RESEARCH PAPERS

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

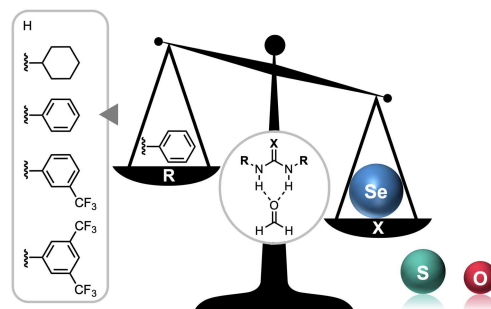
Daisuke Asakura,* Takaaki Sudayama, Yusuke Nanba, Eiji Hosono, Hisao Kiuchi, Kosuke Yamazoe, Jun Miyawaki, Yoshihisa Harada, Atsuo Yamada, Ru-Pan Wang and Frank M. F. de Groot



4099

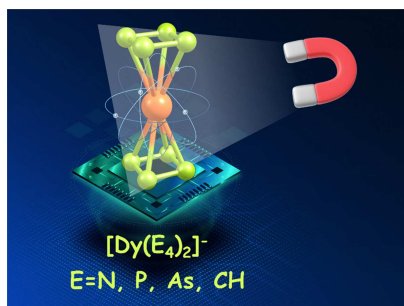
Urea hydrogen-bond donor strengths: bigger is not always better

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



RESEARCH PAPERS

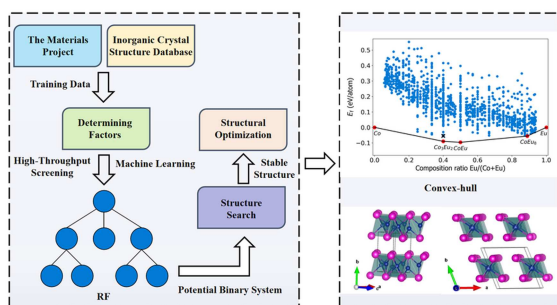
4109



Unravelling the electronic structure, bonding, and magnetic properties of inorganic dysprosocene analogues $[\text{Dy}(\text{E}_4)_2]^-$ (E = N, P, As, CH)

Ibtesham Tarannum and Saurabh Kumar Singh*

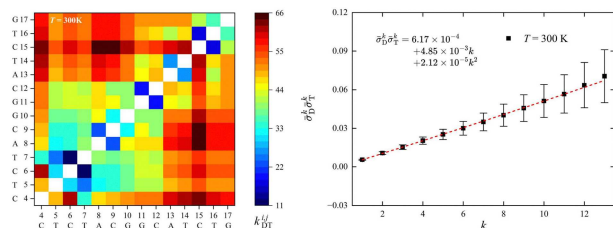
4121



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

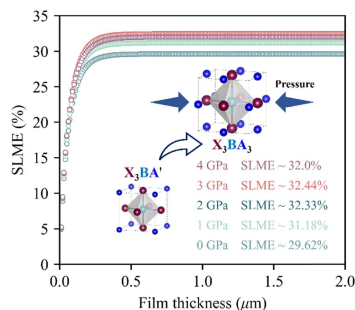
4129



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 X_3AsCl_3 (X = Mg, Ca, Sr, Ba): a first-principles study

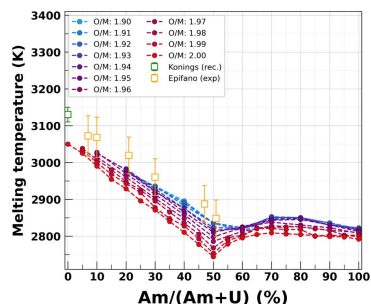
Tao Hu, Changhe Wu, Mingjun Li, Hao Qu, Xin Luo,
Yihao Hou, Shichang Li, Shengnan Duan, Dengfeng Li,*
Gang Tang* and Chunbao Feng*

RESEARCH PAPERS

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

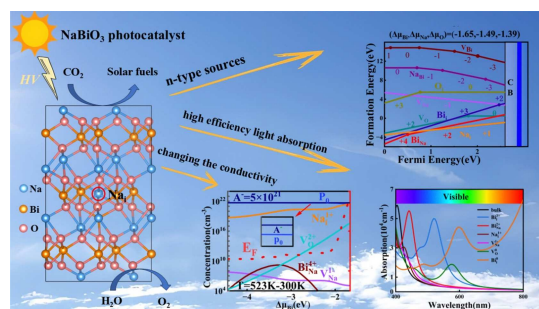
Baptiste Labonne, Christine Guéneau and Marjorie Bertolus*



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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*

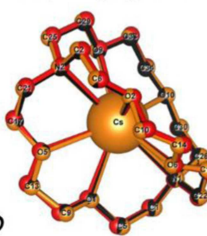
Experimental
 $V=1235 \text{ \AA}^3$
 $\delta_{iso}=225 \text{ ppm}$
 $Cq=1047 \text{ kHz}$

$Cs^+[2.2.2]cryptand$

PBE

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

^{133}Cs DFT/NMR

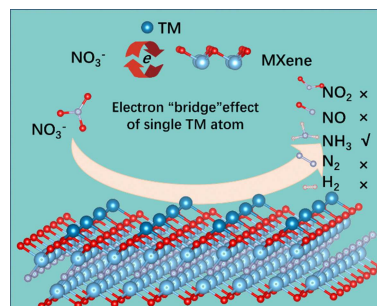


rev-vdW-DF2
 $V=1209 \text{ \AA}^3$
 $\delta_{iso}=228.7 \text{ ppm}$
 $Cq=1071 \text{ kHz}$

4202

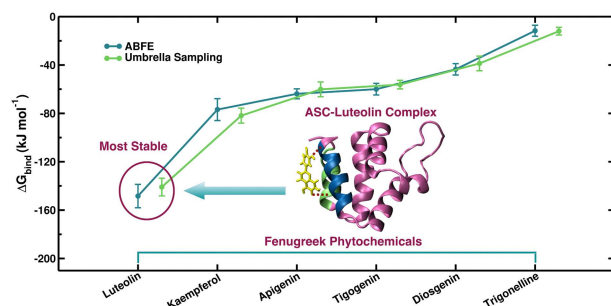
Revealing the origin of activity and selectivity in nitrate to ammonia conversion on single transition metal atom catalysts supported by a Ti_2NO_2 monolayer

Yuwen Cheng,* Wenjie Wang and Cuiping Shao



RESEARCH PAPERS

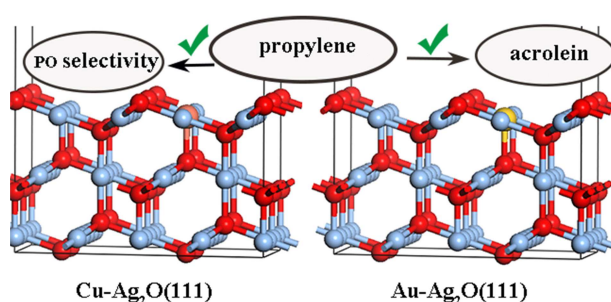
4211



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

Avinash Garg and Ananya Debnath*

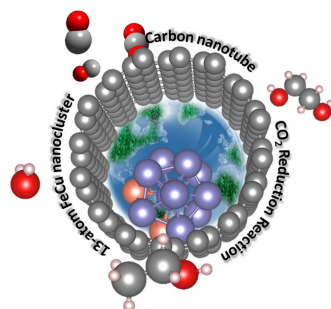
4222



Effect of Cu/Au for propylene epoxidation over the Ag₂O(111) surface: a DFT study

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

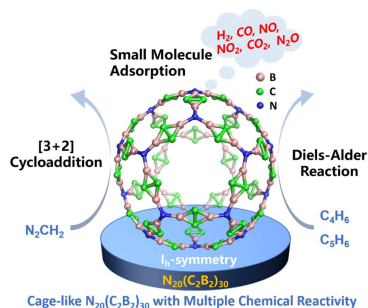
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The roles of various Fe–Cu bimetallic nanoclusters in controlling the C2 selectivity for the CO reduction reaction – a DFT study

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

4246



High-symmetry cage-like molecule N₂₀(C₂B₂)₃₀: computational insight into its bonding and reactivity

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

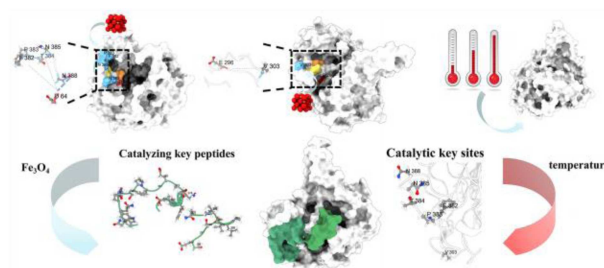


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The effect of the allosteric regulation on the catalytic activity of fructosyltransferase studied via molecular dynamics simulations

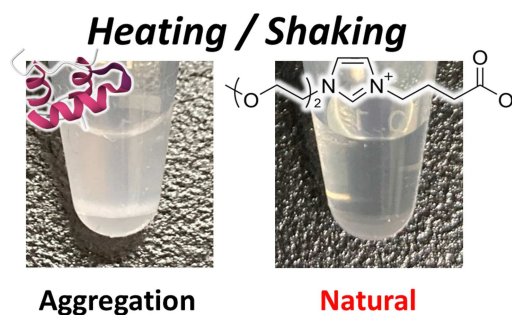
Chaofan Yu, Yanqi Liu, Liang Fu, Zhengyu Shu, Mojie Duan* and Yi Zheng*



4263

Stabilizing protein pharmaceuticals by imidazolium-type zwitterions

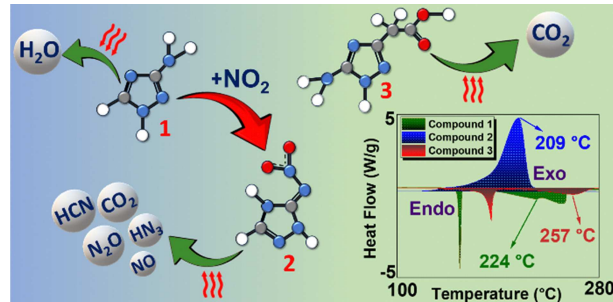
Ai Tajiri, Takeru Ishizaki, Takahiro Takekiyo, Kazuaki Ninomiya, Kenji Takahashi and Kosuke Kuroda*



4269

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

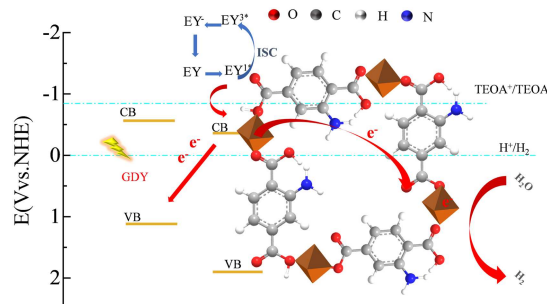
Sarika Venugopal, Shani Saha, Neeraj Kumbhakarna and Anuj A. Vargeese*



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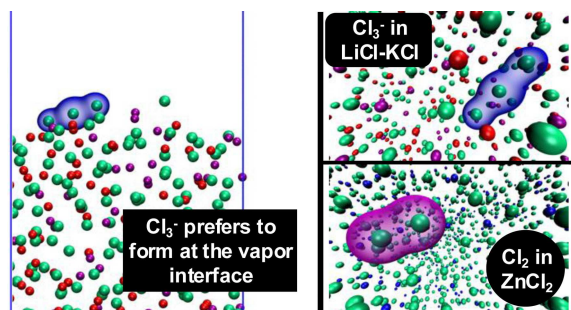
Efficient photocatalytic hydrogen production by employing a graphdiyne/ $\text{NH}_2\text{-MIL-88B(Fe)}$ composite

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



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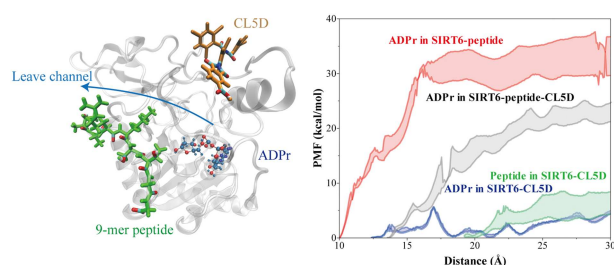
4290



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*

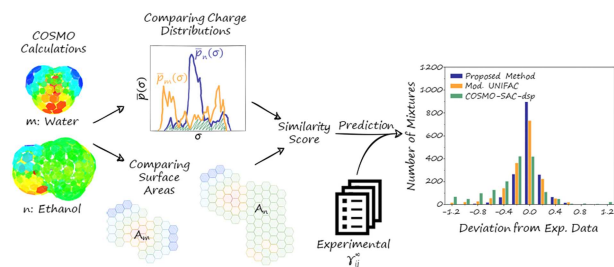
4298



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*

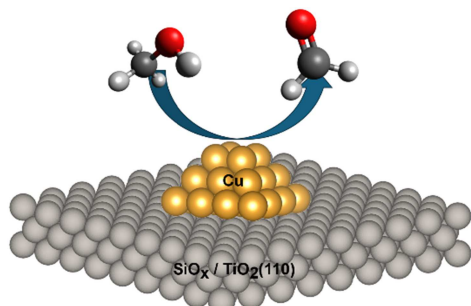
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Prediction of activity coefficients by similarity-based imputation using quantum-chemical descriptors

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*

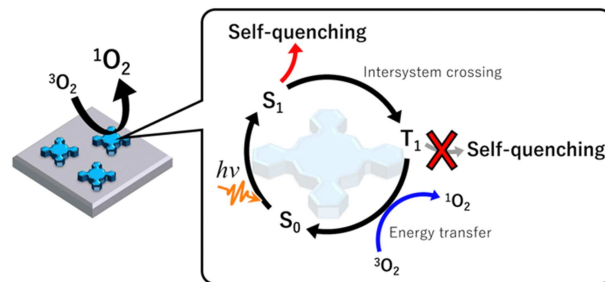


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4328

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

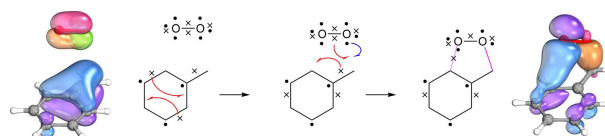
Takuya Fujimura,* Kazuya Okada, Masatoshi Nishiguchi, Yasuyuki Araki, Takahisa Ikeue and Ryo Sasai*



4335

Benzylperoxy radical cation: an exceptionally stable and bound species

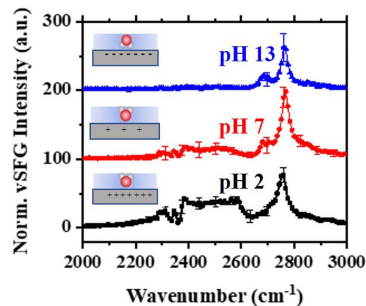
Chow-Shing Lam, Xi-Guang Wei, Yi Pan and Kai-Chung Lau*



4343

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

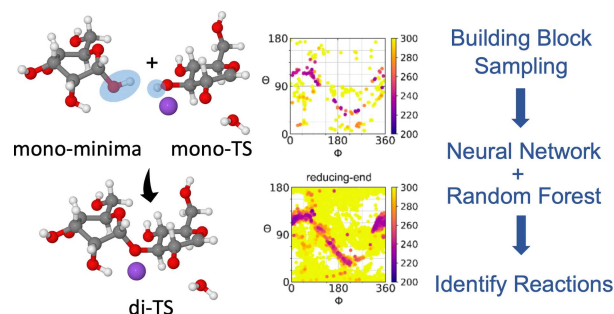
Narendra M. Adhikari,* Piotr Zarzycki, Zheming Wang and Kevin M. Rosso*



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

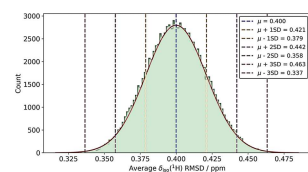
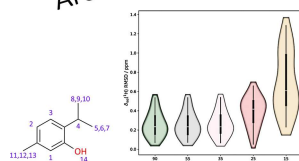
Pei-Kang Tsou, Huu Trong Phan and Jer-Lai Kuo*



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4368

Thymol, Where
Are You????

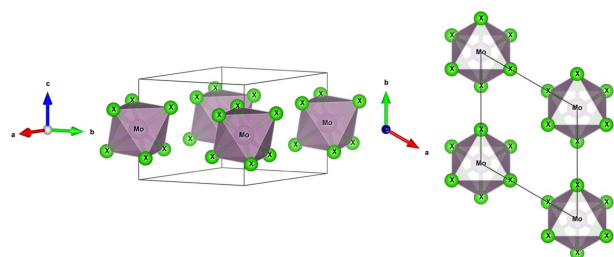


More Efficient
GIPAW DFT ^1H Shifts

^1H isotropic chemical shift metrics for NMR crystallography of powdered molecular organics

Fatemeh Zakeri and Cory M. Widdifield*

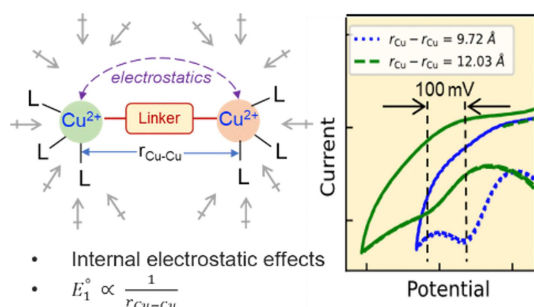
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Exploring the physical properties of the new MoX_6 (X = Cl or Br) materials

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

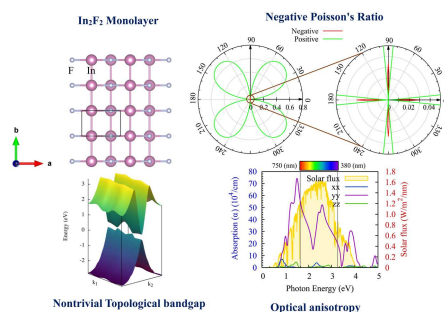
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Influence of internal electrostatics on reduction potentials in amine-ligated bimetallic copper complexes

Prateek Saini, Shubham Gupta and Srinivasan Ramakrishnan*

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In_2F_2 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

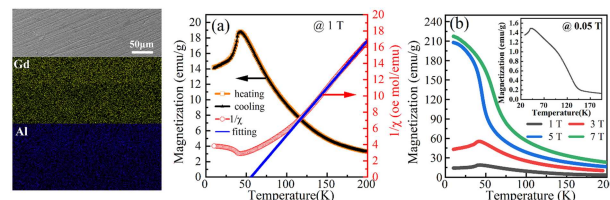


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First-order non-hysteretic phase transition: a pathway to enhanced magnetocaloric and giant magnetoresistance effects in a Gd–Al alloy

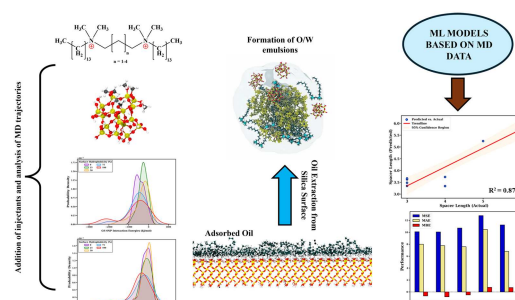
Guiquan Yao, Peng Gao, Zonghang Liu,* Che Zhang,* Guangzhao Wang and Weibin Cui*



4429

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

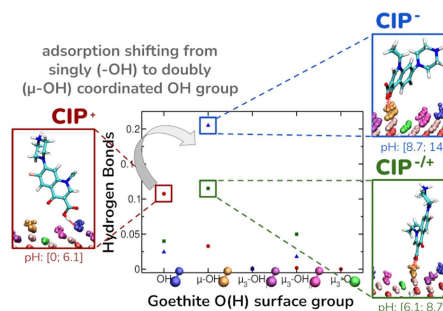
Gourav Chakraborty, Keka Ojha, Ajay Mandal and Niladri Patra*



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

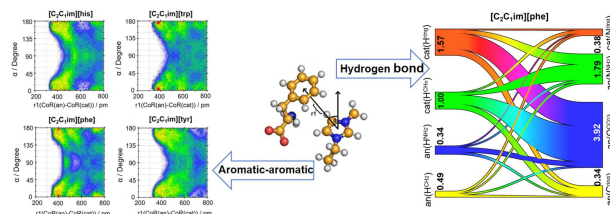
Sébastien Le Crom* and Jean-François Boily*



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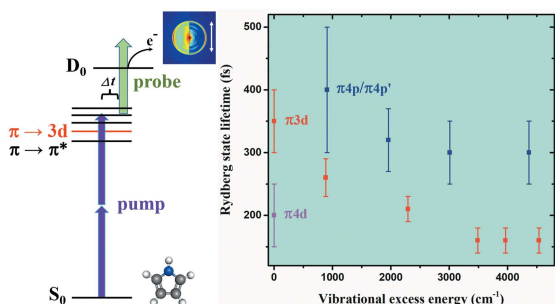
Aromatic–aromatic interactions and hydrogen bonding in amino acid based ionic liquids

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



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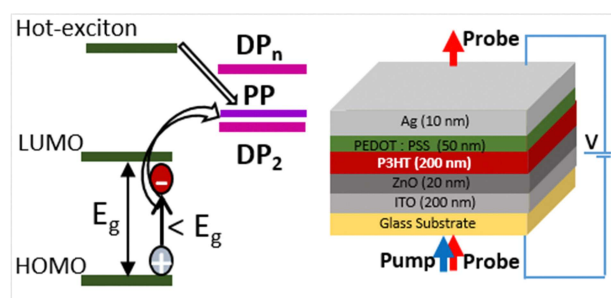
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Time-resolved measurements of subpicosecond excited-state lifetimes of high-lying Rydberg states in pyrrole

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

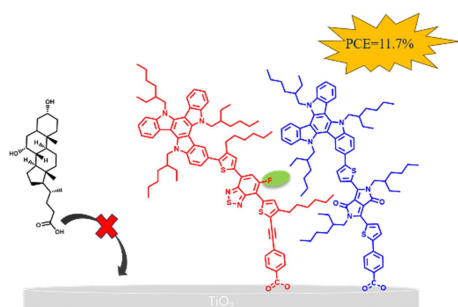
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Direct route of ultrafast charge-pair generation upon below-band-gap excitation in P3HT: effect of external electric field

Debkumar Rana,* Ayush Kant Ranga and Arnulf Materny*

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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*

