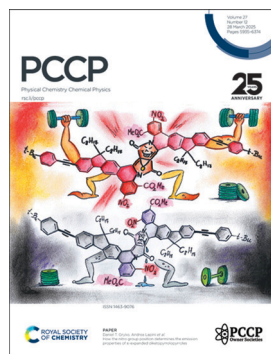


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ISSN 1463–9076 CODEN PPCPFQ 27(12) 5935–6374 (2025)



Cover

See Daniel T. Gryko, Andrea Lapini *et al.*, pp. 5965–5972. Image reproduced by permission of Daniel T. Gryko from *Phys. Chem. Chem. Phys.*, 2025, 27, 5965. Image designed by Dominika Bednarska.



Inside cover

See Alexandra Wahab and Renana Gershoni-Poranne, pp. 5973–5983. Image reproduced by permission of Renana Gershoni-Poranne from *Phys. Chem. Chem. Phys.*, 2025, 27, 5973.

COMMUNICATIONS

5949

An archetype of hydrogen bonding observed in cationic dimers of carboxy-functionalized ionic liquids by means of NMR solid state spectroscopy – reminiscent of salt bridges, peptides and DNA

Alexander E. Khudozhitkov, Lasse Hunger, Loai Al-Sheakh, Alexander G. Stepanov, Daniil I. Kolokolov* and Ralf Ludwig*

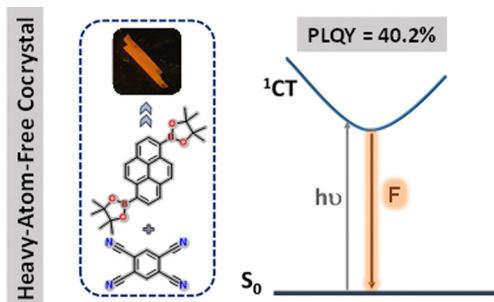
Curious Hydrogen Bond Strength



5956

Harnessing luminescence from a heavy-atom-free organic charge-transfer cocrystal

Suvarna Sujilkumar and Mahesh Hariharan*



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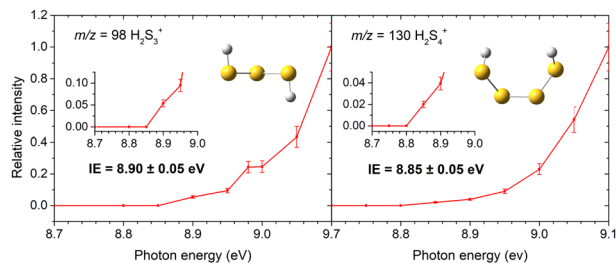


COMMUNICATIONS

5961

An experimental and theoretical study of the photoionization properties of polysulfanes (H_2S_n , $n = 2-4$)

Zhibiao Li, Jianchao Yang, Xinyue Gong, Weijun Zheng, Chongqin Zhu* and Cheng Zhu*

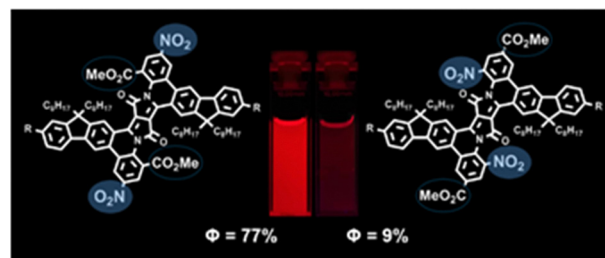


RESEARCH PAPERS

5965

How the nitro group position determines the emission properties of π -expanded diketopyrrolopyrroles

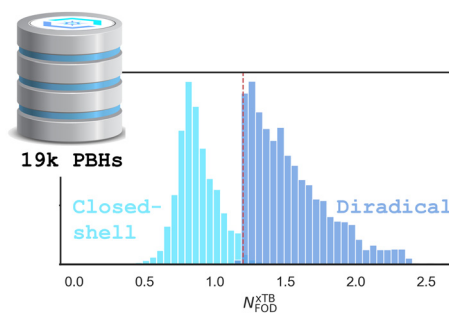
Kamil Skonieczny, Francesco Di Maiolo, Sara Venturi, Alessandro Iagatti, Alessandro Ricci, Francesco Bertocchi, Daniel T. Gryko* and Andrea Lapini*



5973

Accelerated diradical character assessment in large datasets of polybenzenoid hydrocarbons using xTB fractional occupation

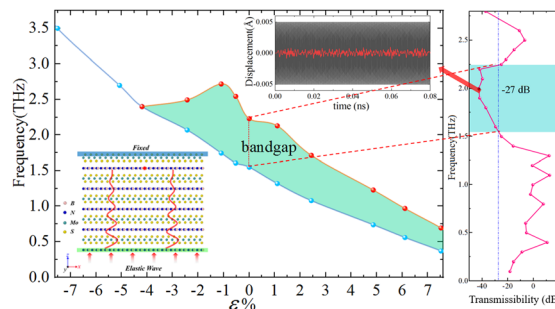
Alexandra Wahab and Renana Gershoni-Poranne*



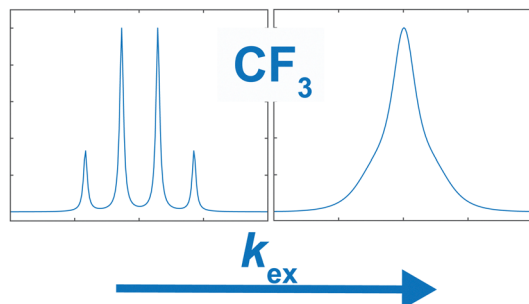
5984

Tunable elastic wave bandgaps by strain engineering of multilayered van der Waals metamaterials

Yabin Jing, Lifeng Wang* and Eric Li



5995

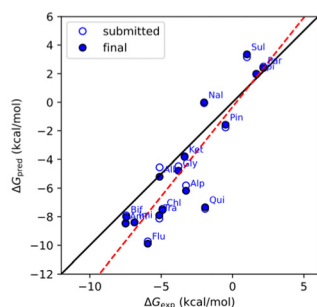
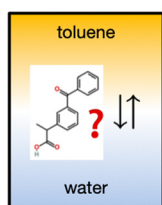


The influence of fluorine spin-diffusion on ^{13}C solid-state NMR line shapes of CF_3 groups

Ettore Bartalucci, Calogero Quaranta, Fabio Manzoni, Igor d'Anciães Almeida Silva, Mirijam Zobel, Carsten Bolm, Matthias Ernst* and Thomas Wiegand*

6005

SAMPL9 logP challenge

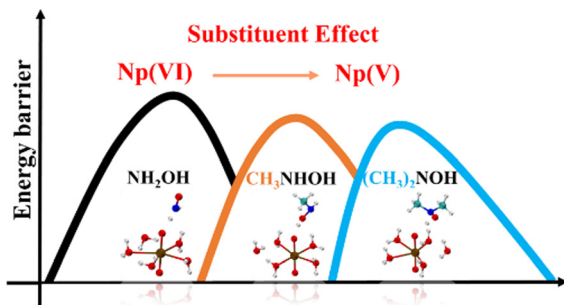


Expanded Ensemble (EE) MD + OpenFF 2.0.0

Expanded ensemble predictions of toluene–water partition coefficients in the SAMPL9 log P challenge

Steven R. Goad, Robert M. Raddi and Vincent A. Voelz*

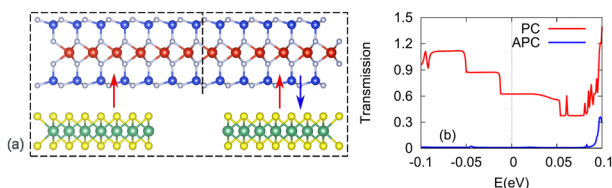
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Theoretical study on the kinetic behavior of $\text{Np}(\text{VI})$ reduction by hydroxylamine and its derivatives: substituent effect

Xin Huang, Qun-Yan Wu,* Cong-Zhi Wang, Jian-Hui Lan, Hong-Qing Wang* and Wei-Qun Shi*

6024



Tuning the conducting types of VSi_2N_4 by van der Waals engineering

Wenlin Li, Xiaohong Zheng,* Chun-Sheng Liu, Hua Hao,* Weiyang Wang* and Yushen Liu

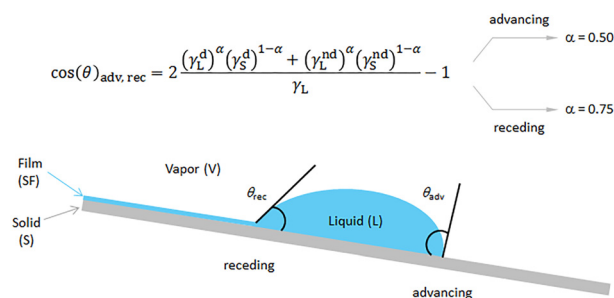


RESEARCH PAPERS

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Estimating advancing and receding contact angles for pure and mixed liquids on smooth solid surfaces using the PCP-SAFT equation of state

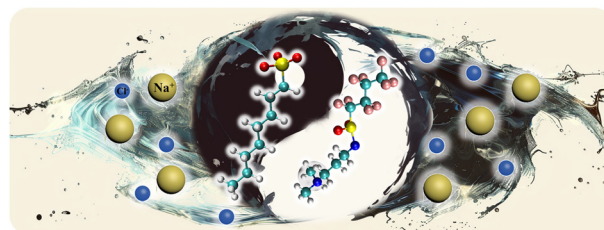
Aliakbar Roosta,* Sohrab Zendeboudi and Nima Rezaei



6043

Molecular dynamics simulation of synergistic behavior at the air–water interface: mixed cationic–anionic fluorocarbon–hydrocarbon surfactants

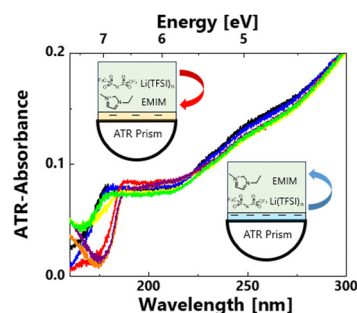
Xiaolong Quan, Jing Xiong, Tong Tong, Jinqing Jiao,* Jianping Zou and Yuechang Wei*



6056

Molecular insight into the dynamics at the lithium-containing ionic liquid/gold film electrode interface using electrochemical attenuated total reflection spectroscopies

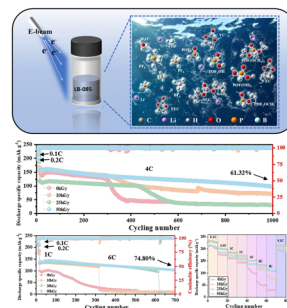
Tomonori Kakinoki,* Akihito Imanishi, Shinji Kondou, Ichiro Tanabe and Ken-ichi Fukui*



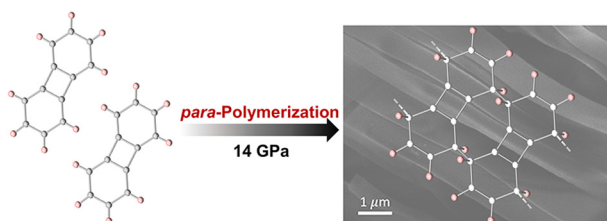
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High energy electron beam irradiation on the electrolyte enables fast-charging of lithium metal batteries with long-term cycling stability

Miaomiao Yu, Qiaoan Liu, Yuxin Rao, Huasong Wang, Pengfei Liu, Xue Li, Yan Zhang* and Shan Fang*



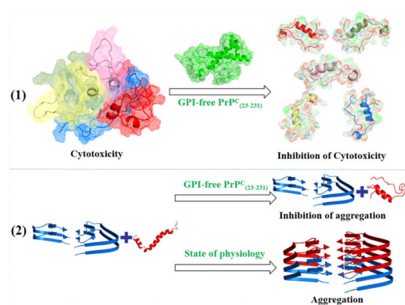
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Synthesis of a biphenylene nanoribbon by compressing biphenylene under extreme conditions

Zilin Zhao, Guangwei Che, Fang Li, Yunfan Fei, Hao Luo, Puyi Lang, Qingchao Zeng, Hongcun Bai, Yajie Wang,* Ho-kwang Mao, Haiyan Zheng* and Kuo Li*

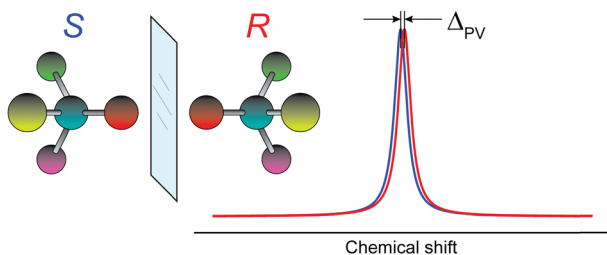
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Deciphering the full-length PrP^C_(23–231) receptor and characterizing the size/subphase-dependent impact of Aβ oligomers on the PrP^C_(23–231) receptor: insights from molecular dynamics simulations

Chuanbo Wang, Mengke Jia, Yvning Guan, Sajjad Ahmad, Jinfei Mei* and Hongqi Ai*

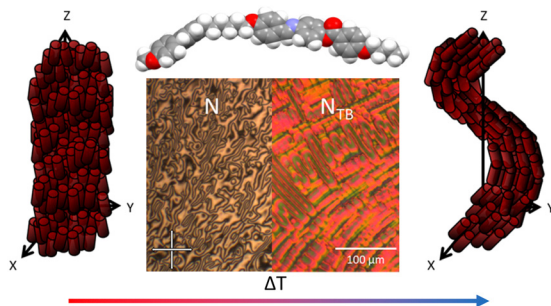
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Towards detection of molecular parity violation via chiral co-sensing: the ¹H/³¹P model system

Erik Van Dyke, James Eills, Kirill Sheberstov, John Blanchard, Manfred Wagner, Andrés Emilio Wedenig, Konstantin Gaul,* Robert Berger, Rudolf Pietschnig, Denis Kargin, Danila A. Barskiy* and Dmitry Budker*

6104



Twist-bend liquid crystal phases and molecular structure: the role of methoxybiphenyl

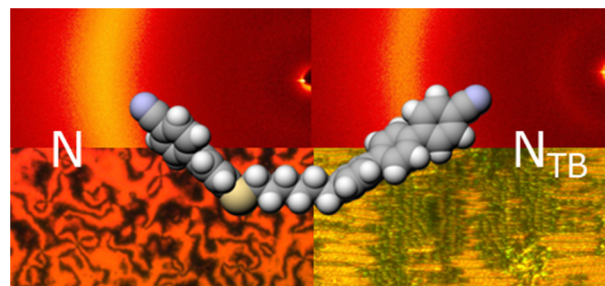
Calum J. Gibb,* Magdalena M. Majewska, Grant J. Strachan, Damian Pocięcha, John M. D. Storey,* Ewa Gorecka and Corrie T. Imrie



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Sulfur-linked cyanoterphenyl-based liquid crystal dimers and the twist-bend nematic phase

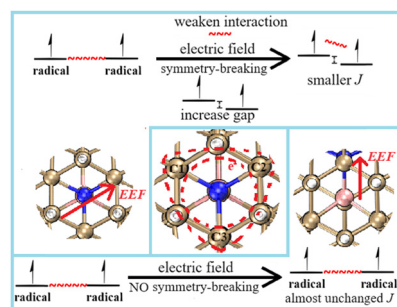
Ewan Cruickshank,* Grant J. Strachan, Abigail Pearson, Damian Pocięcha, Ewa Gorecka, John M. D. Storey and Corrie T. Imrie



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Electric field manipulated magnetic spin coupling properties in lithium-trapped nitrogen-vacancy nanodiamonds

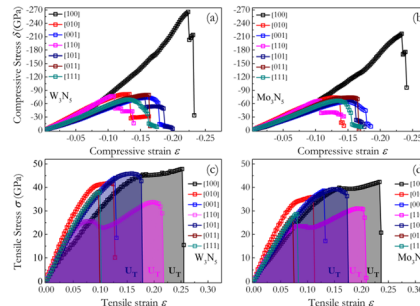
Zhuxiao Li, Zhiru Zhang, Yuxiang Bu and Xinyu Song*



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Structural, strength and fracture mechanisms of superconducting transition metal nitrides TM_3N_5 (TM = W and Mo)

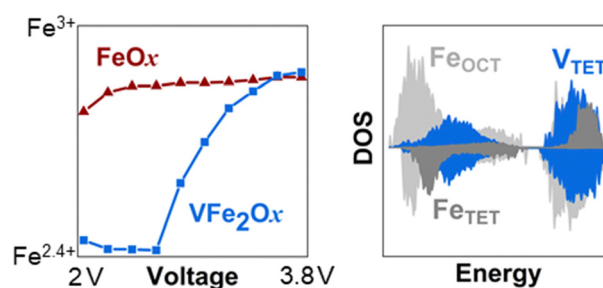
Haiyan Yan, Wenhui Zhang, Lei Chen, Yun Zhang, Hui Wang, Meiguang Zhang* and Qun Wei*



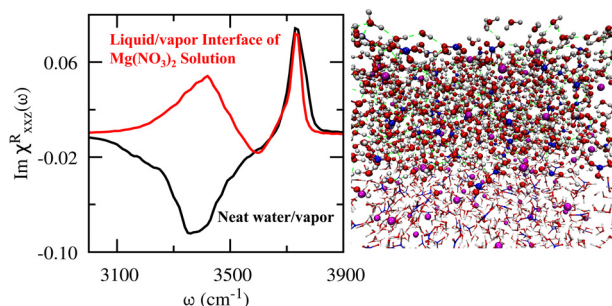
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Deconvolving lithium-ion redox in vanadium–iron oxide aerogels using X-ray absorption spectroscopy and density functional theory

Ryan H. DeBlock, Michelle D. Johannes, Hunter O. Ford, Michael W. Swift, Debra R. Rolison and Jeffrey W. Long*



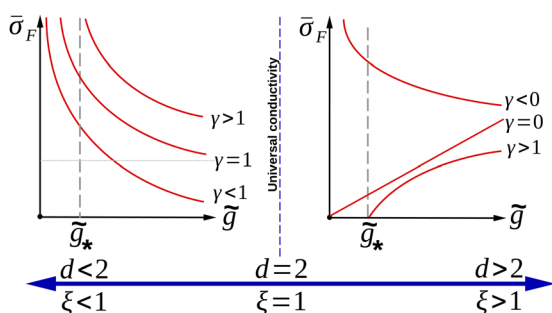
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Effects of cations on the structure, dynamics and vibrational sum frequency generation spectroscopy of liquid/vapor interfaces of aqueous solutions of monovalent and divalent metal nitrates

Abhilash Chandra, Shinji Saito* and Amalendu Chandra*

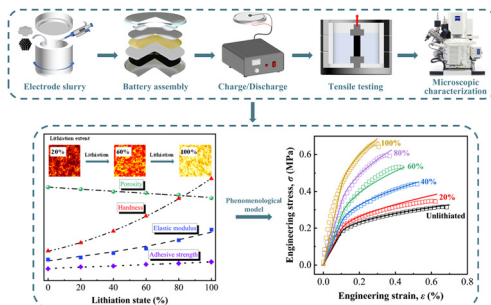
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Disorder driven peculiarities of metal-insulator transition in the interacting fermions ensemble

A. Sinner,* V. A. Stephanovich, E. V. Kirichenko and K. Książek

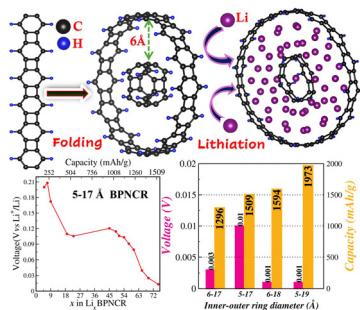
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Revealing the mechanical behaviour and material micro-structure of graphite electrode coatings in lithium-ion batteries during lithiation

Detao Kong, Liang Fu, Qinghua Yang, Yaolong He* and Hongjiu Hu*

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Biphenylene concentric nanorings as high-performance anode materials for lithium-ion batteries: a DFT-based study on lithium intercalation and capacity enhancement

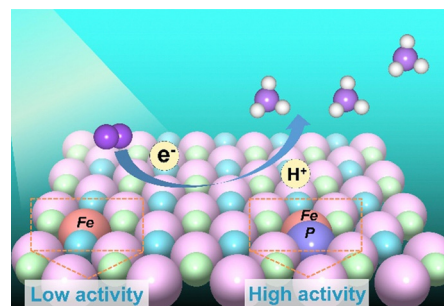
Zubair Nabi Ganaie and Priya Johari*



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Regulating the spin state of a single Fe atom in BiOBr to enhance photocatalytic nitrogen reduction: insights from theoretical studies

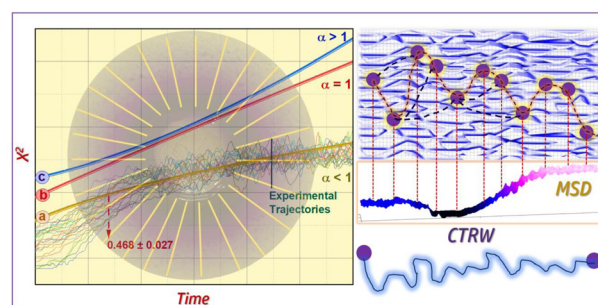
Zhanjin Wang, Xiao Han and Jinlu He*



6212

Concentration-dependent anomalous diffusion of crystal violet dye in agar gel: application of the continuous time random walk model

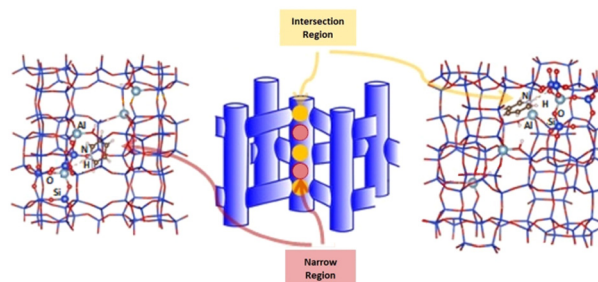
Rachana D. Bamb, Prasad C. Walimbe, Sunil D. Kulkarni* and Preeti S. Kulkarni*



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A comparative theoretical study of cluster and periodic models by DFT calculations for pyridine adsorption in H-ZSM-5 zeolite

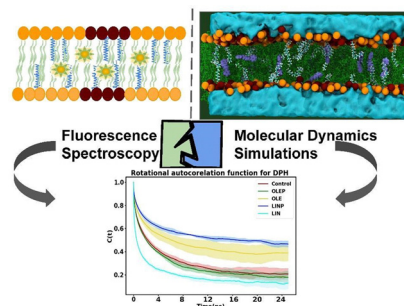
E. Kassab* and M. Castellà-Ventura



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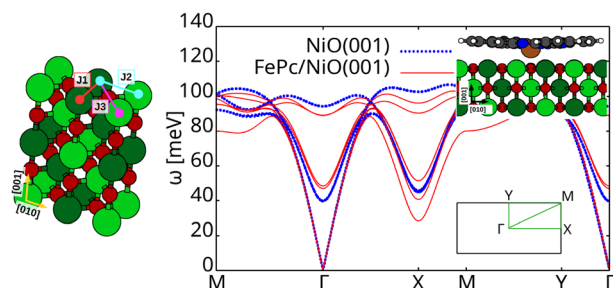
Anomalous membrane organization by omega-6 and omega-9 fatty acids

Sudha Porte, Swaratmika Pandia, Ankita Joardar, Deepashri Saraf, Aadil Pinjari, Hiral Chakraborty* and Durba Sengupta*



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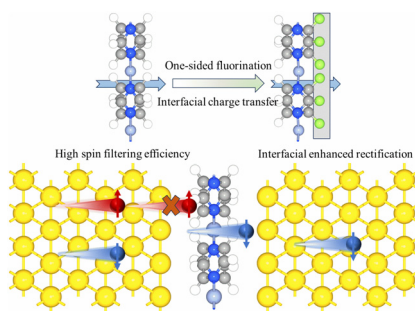
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Chemical tuning of magnons in NiO(001) by Fe-phthalocyanine adsorption

Marco Marino,* Gonzalo Rivero-Carracedo, Andrey Rybakov, José J. Baldoví* and Guido Fratesi

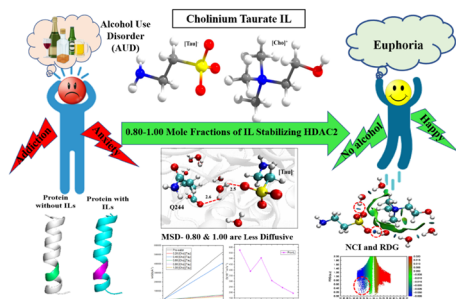
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Interface-driven spin filtering and diode effects in van der Waals junctions based on magnetic metal–organic frameworks

Mingqiang Ge, Ziqiang Liu, Tong Chen, Liang Xu and Lin Huang*

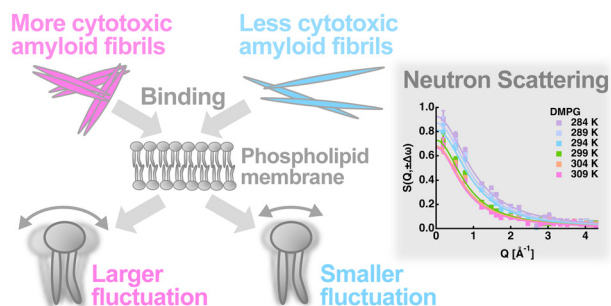
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Molecular mechanism behind the cholinium-taurate ionic liquid in stabilisation of HDAC2 for alcohol use disorders: insights from DFT and MD simulations

S. M. Esther Rubavathy, Gopal Hema and Muthuramalingam Prakash*

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Sub-nanosecond dynamics of phospholipid membranes interacting with polymorphic amyloid fibrils observed by elastic incoherent neutron scattering

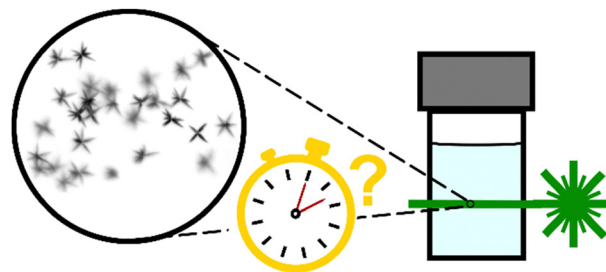
Tatsuhito Matsuo,* Agathe Bélimé, Francesca Natali, Alessio De Francesco and Judith Peters*



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High-speed imaging of non-photochemical laser-induced nucleation in aqueous cesium chloride

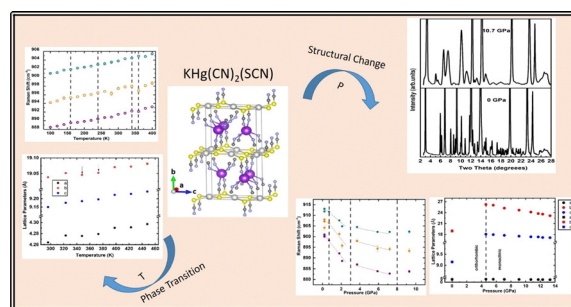
Eleanor R. Barber and Andrew J. Alexander*



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Thermal and pressure response of $\text{KHg}(\text{CN})_2(\text{SCN})$

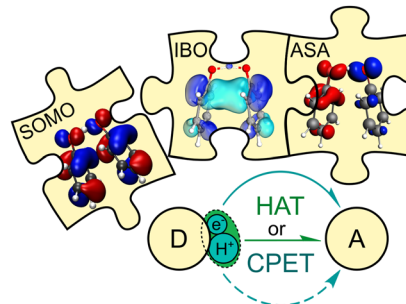
Aashna Jain, Pallavi Ghalsasi,* Srinu Tothadi, Nandini Garg, Alka B. Garg, Prafulla K. Jha, Hemant Mande and Prasanna S. Ghalsasi*



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Concerted proton electron transfer or hydrogen atom transfer? an unequivocal strategy to discriminate these mechanisms in model systems

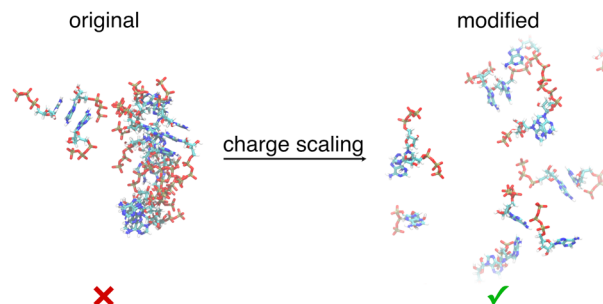
Davide Zeppilli and Laura Orian*



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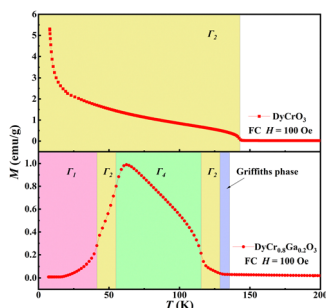
Development of a force field for ATP – how charge scaling controls self-association

Tuan Minh Do,* Nobuyuki Matubayasi and Dominik Horinek*



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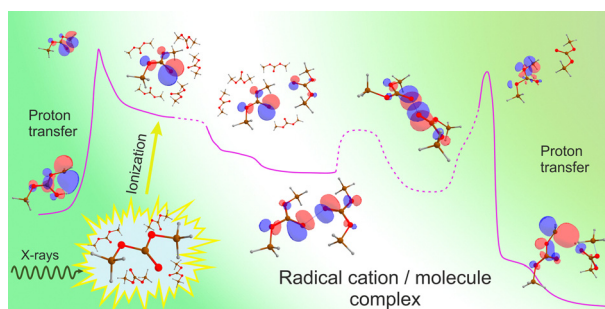
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Multiple spin reorientation transitions in Ga^{3+} -substituted DyCrO_3

Xiong-Han Liu, Meng-Qi Ye, Hai-Bo Xiao,*
Shi-Heng Liang, Zheng-Cai Xia and Rui-Long Wang*

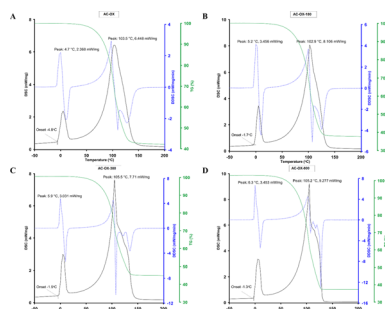
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Primary radical ions in irradiated carbonates

Irina S. Tretyakova and Vsevolod I. Borovkov*

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The influence of surface chemistry of activated carbons on adsorption and freezing/melting processes

Alicja Bosacka,* Małgorzata Zienkiewicz-Strzałka,
Anna Deryto-Marczewska,* Agnieszka Chrzanowska,
Małgorzata Wasilewska and Piotr Pikuta

CORRECTION

6372

Correction: Electronic structure, absorption spectra and oxidation dynamics in polyynes and dicyanopolyynes

Lazaros Chalkopiadis, Konstantinos Lambropoulos and Constantinos Simserides*

