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### IN THIS ISSUE

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#### Cover

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Andrea Lapini et al.,  
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#### Inside cover

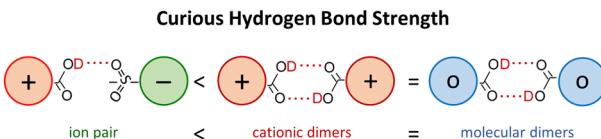
See Alexandra Wahab  
and Renana Gershoni-  
Poranne, pp. 5973–5983.  
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*Phys. Chem. Chem. Phys.*,  
2025, 27, 5973.

### 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

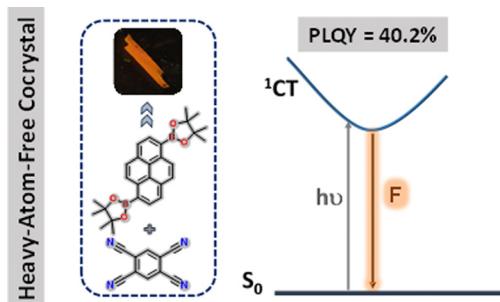
Alexander E. Khudozhitkov, Lasse Hunger,  
Loai Al-Sheakh, Alexander G. Stepanov,  
Daniil I. Kolokolov\* and Ralf Ludwig\*



5956

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

Suvarna Sujilkumar and Mahesh Hariharan\*





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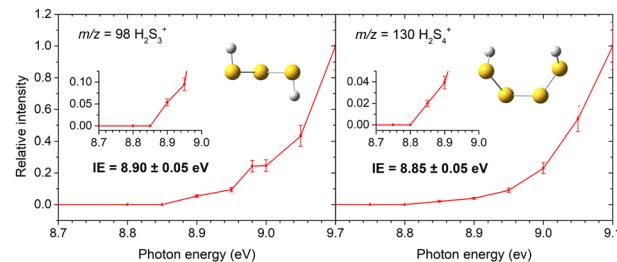


## COMMUNICATIONS

5961

**An experimental and theoretical study of the photoionization properties of polysulfanes ( $\text{H}_2\text{S}_n$ ,  $n = 2-4$ )**

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

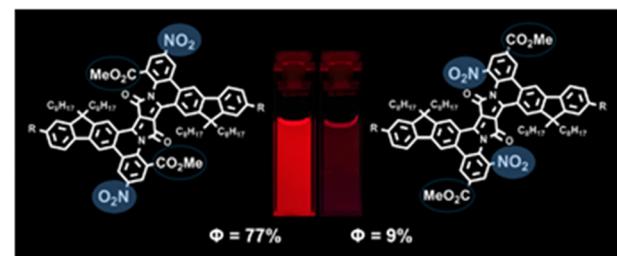


## RESEARCH PAPERS

5965

**How the nitro group position determines the emission properties of  $\pi$ -expanded diketopyrrolopyrroles**

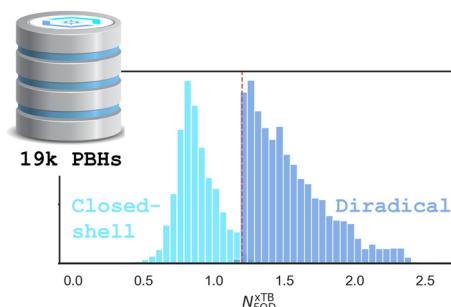
Kamil Skonieczny, Francesco Di Maiolo, Sara Venturi, Alessandro Iagatti, Alessandro Ricci, Francesco Bertocchi, Daniel T. Gryko\* and Andrea Lapini\*



5973

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

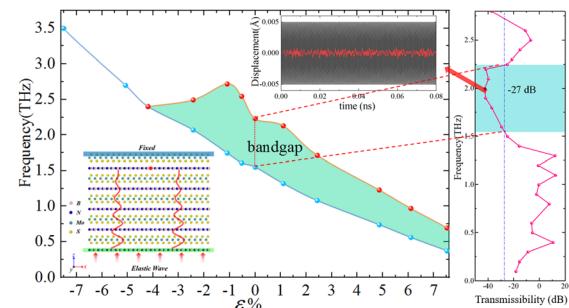
Alexandra Wahab and Renana Gershoni-Poranne\*



5984

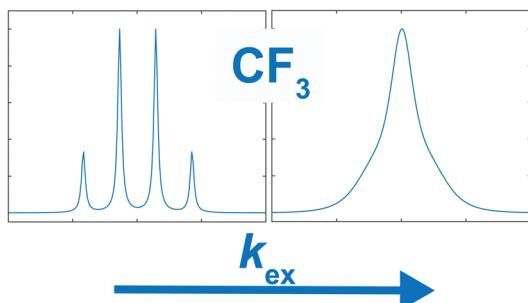
**Tunable elastic wave bandgaps by strain engineering of multilayered van der Waals metamaterials**

Yabin Jing, Lifeng Wang\* and Eric Li



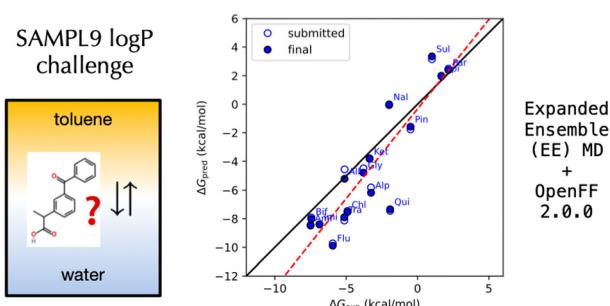
## RESEARCH PAPERS

5995

**The influence of fluorine spin-diffusion on  $^{13}\text{C}$  solid-state NMR line shapes of  $\text{CF}_3$  groups**

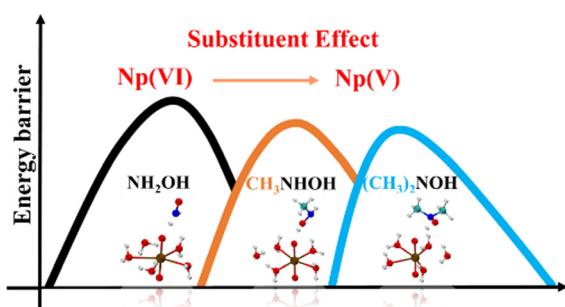
Ettore Bartalucci, Calogero Quaranta, Fabio Manzoni, Igor d'Anci  es Almeida Silva, Mirijam Zobel, Carsten Bolm, Matthias Ernst\* and Thomas Wiegand\*

6005

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

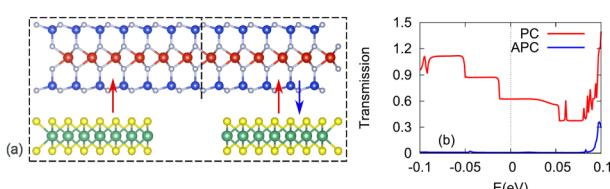
Steven R. Goold, Robert M. Raddi and Vincent A. Voelz\*

6014

**Theoretical study on the kinetic behavior of  $\text{Np(VI)}$  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  $\text{VSi}_2\text{N}_4$  by van der Waals engineering**

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



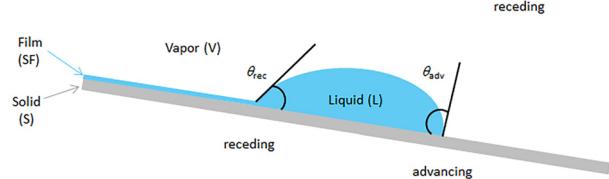
## RESEARCH PAPERS

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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 Zendehboudi and Nima Rezaei

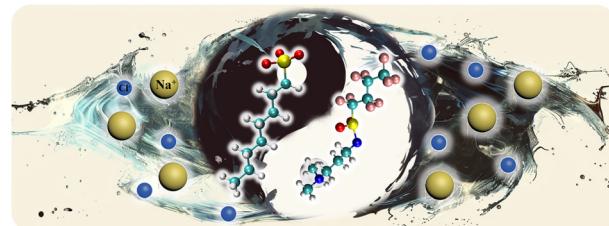
$$\cos(\theta)_{\text{adv}, \text{rec}} = 2 \frac{(\gamma_L^d)^\alpha (\gamma_S^d)^{1-\alpha} + (\gamma_L^{\text{nd}})^\alpha (\gamma_S^{\text{nd}})^{1-\alpha}}{\gamma_L} - 1$$



6043

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

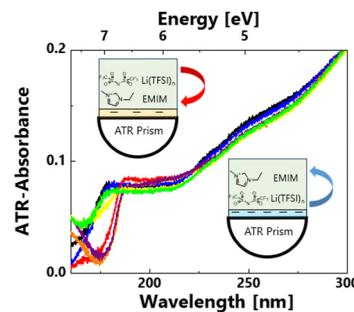
Xiaolong Quan, Jing Xiong, Tong Tong, Jinqing Jiao,\* Jianping Zou and Yuechang Wei\*



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

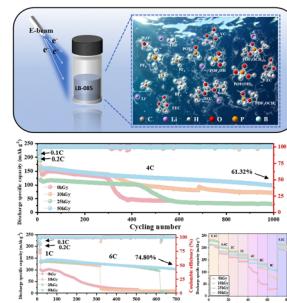
Tomonori Kakinoki,\* Akihito Imanishi, Shinji Kondou, Ichiro Tanabe and Ken-ichi Fukui\*



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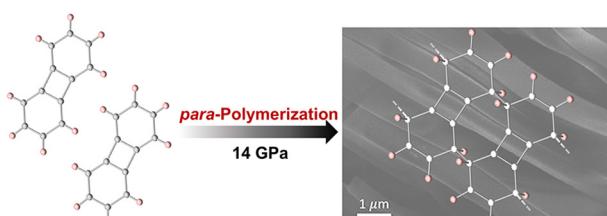
**High energy electron beam irradiation on the electrolyte enables fast-charging of lithium metal batteries with long-term cycling stability**

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



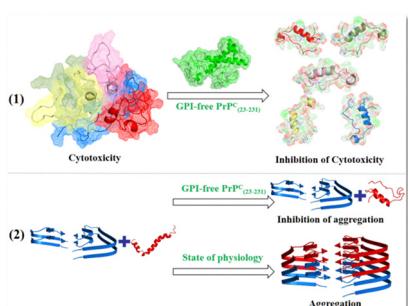
## RESEARCH PAPERS

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**Synthesis of a biphenylene nanoribbon by compressing biphenylene under extreme conditions**

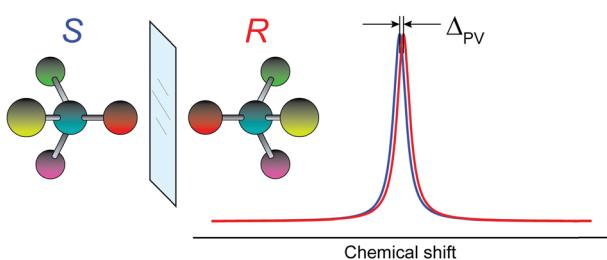
Zilin Zhao, Guangwei Che, Fang Li, Yunfan Fei, Hao Luo, Puyi Lang, Qingchao Zeng, Hongcun Bai, Yajie Wang,\* Ho-kwang Mao, Haiyan Zheng\* and Kuo Li\*

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**Deciphering the full-length PrP<sup>C<sub>(23-231)</sub></sup> receptor and characterizing the size/subphase-dependent impact of A<sub>β</sub> oligomers on the PrP<sup>C<sub>(23-231)</sub></sup> receptor: insights from molecular dynamics simulations**

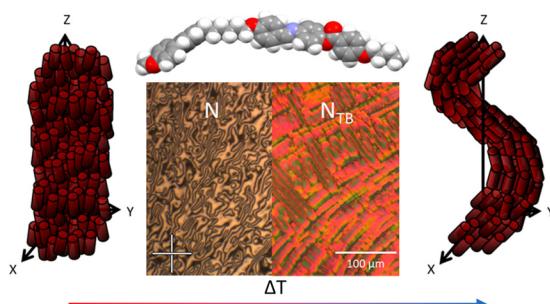
Chuanbo Wang, Mengke Jia, Yvning Guan, Sajjad Ahmad, Jinfei Mei\* and Hongqi Ai\*

6092

**Towards detection of molecular parity violation via chiral co-sensing: the <sup>1</sup>H/<sup>31</sup>P 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 Pociecha, John M. D. Storey,\* Ewa Gorecka and Corrie T. Imrie

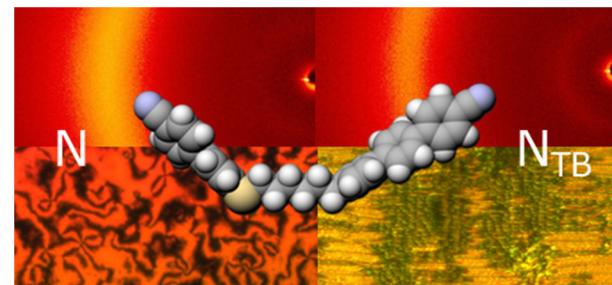


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**Sulfur-linked cyanoterphenyl-based liquid crystal dimers and the twist-bend nematic phase**

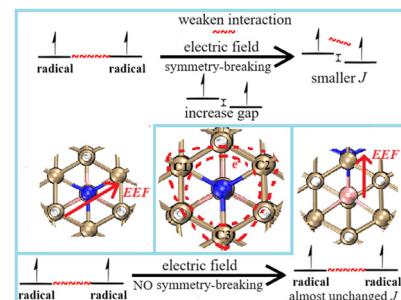
Ewan Cruickshank,\* Grant J. Strachan, Abigail Pearson, Damian Pociecha, Ewa Gorecka, John M. D. Storey and Corrie T. Imrie



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

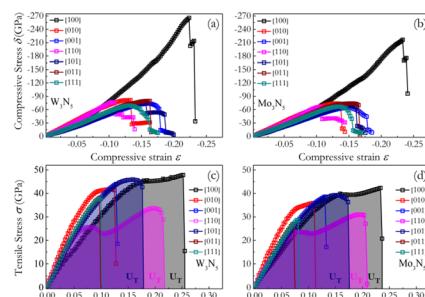
Zhuxiao Li, Zhiru Zhang, Yuxiang Bu and Xinyu Song\*



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**Structural, strength and fracture mechanisms of superconducting transition metal nitrides  $\text{TM}_3\text{N}_5$  ( $\text{TM} = \text{W}$  and  $\text{Mo}$ )**

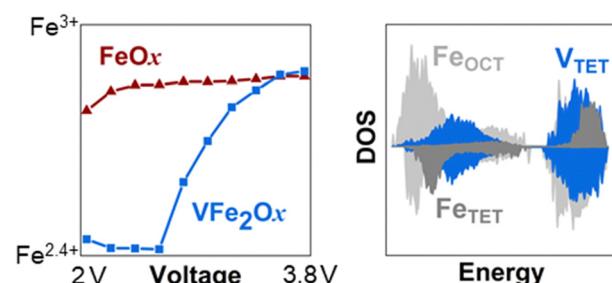
Haiyan Yan, Wenhui Zhang, Lei Chen, Yun Zhang, Hui Wang, Meiguang Zhang\* and Qun Wei\*



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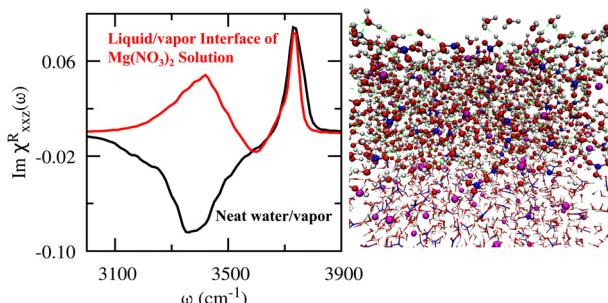
**Deconvolving lithium-ion redox in vanadium–iron oxide aerogels using X-ray absorption spectroscopy and density functional theory**

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



## RESEARCH PAPERS

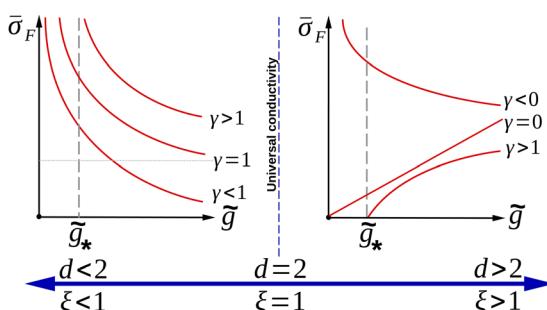
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### Effects of cations on the structure, dynamics and vibrational sum frequency generation spectroscopy of liquid/vapor interfaces of aqueous solutions of monovalent and divalent metal nitrates

Abhilash Chandra, Shinji Saito\* and Amalendu Chandra\*

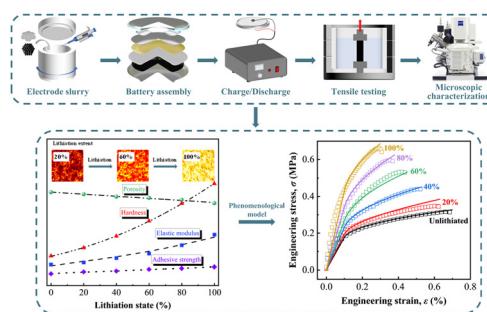
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### Disorder driven peculiarities of metal–insulator transition in the interacting fermions ensemble

A. Sinner,\* V. A. Stephanovich, E. V. Kirichenko and K. Ksiazek

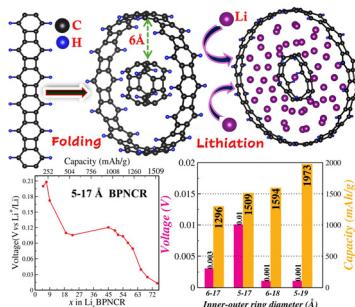
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### Revealing the mechanical behaviour and material micro-structure of graphite electrode coatings in lithium-ion batteries during lithiation

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\*

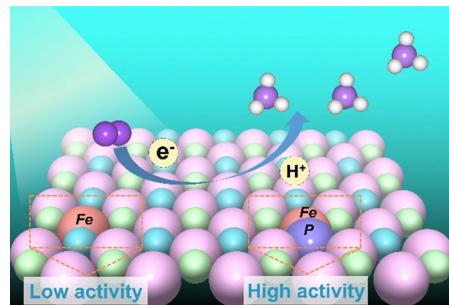


## RESEARCH PAPERS

6205

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

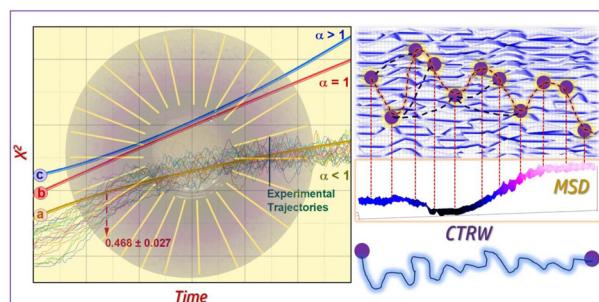
Zhanjin Wang, Xiao Han and Jinlu He\*



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

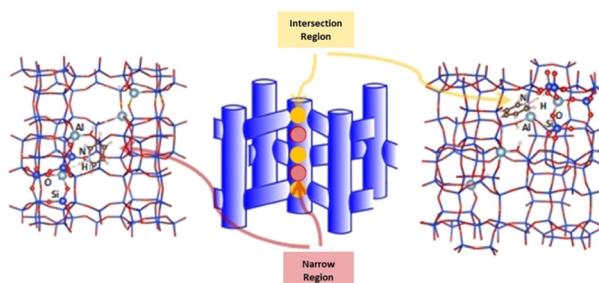
Rachana D. Bamb, Prasad C. Walimbe, Sunil D. Kulkarni\* and Preeti S. Kulkarni\*



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

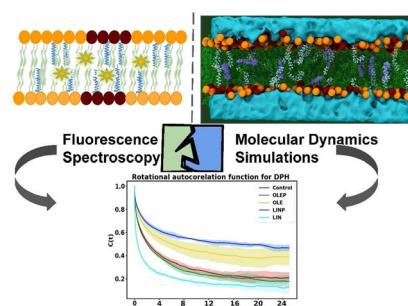
E. Kassab\* and M. Castellà-Ventura



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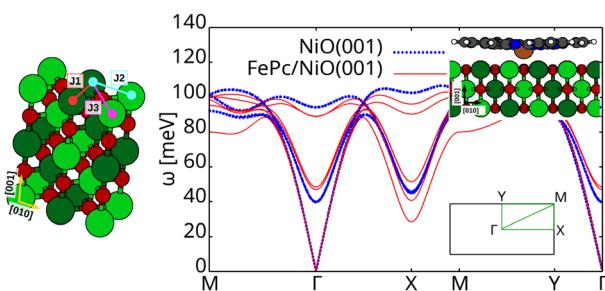
**Anomalous membrane organization by omega-6 and omega-9 fatty acids**

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



## RESEARCH PAPERS

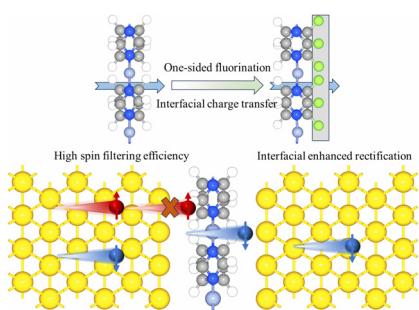
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### Chemical tuning of magnons in NiO(001) by Fe-phthalocyanine adsorption

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

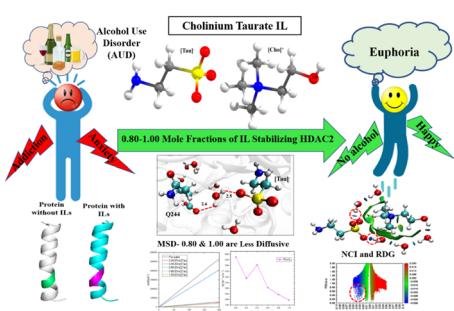
6255



### 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\*

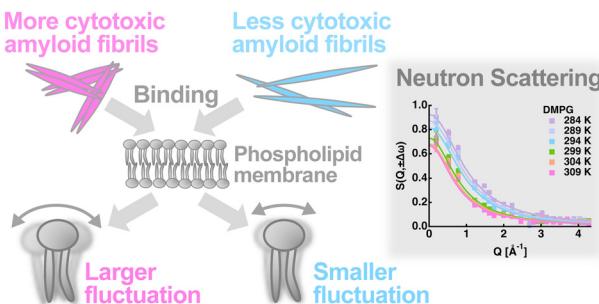
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### Molecular mechanism behind the cholinium-taurate ionic liquid in stabilisation of HDAC2 for alcohol use disorders: insights from DFT and MD simulations

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 Bélime, Francesca Natali, Alessio De Francesco and Judith Peters\*

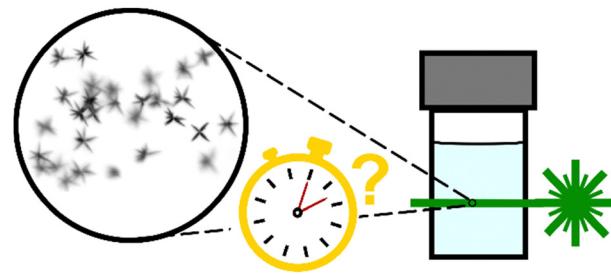


## RESEARCH PAPERS

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

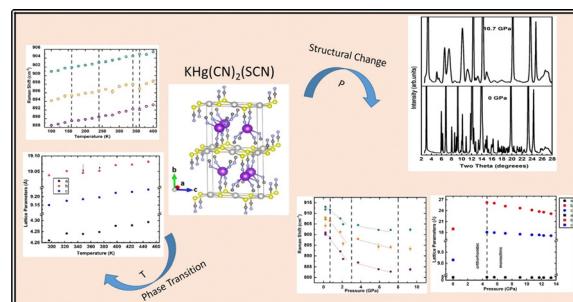
Eleanor R. Barber and Andrew J. Alexander\*



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

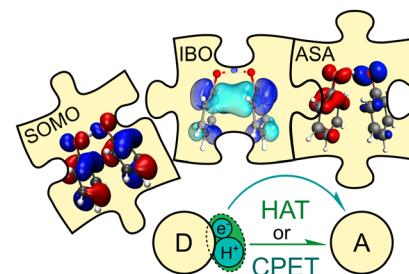
Aashna Jain, Pallavi Ghalsasi,\* Srinu Tothadi, Nandini Garg, Alka B. Garg, Prafulla K. Jha, Hemant Mande and Prasanna S. Ghalsasi\*



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

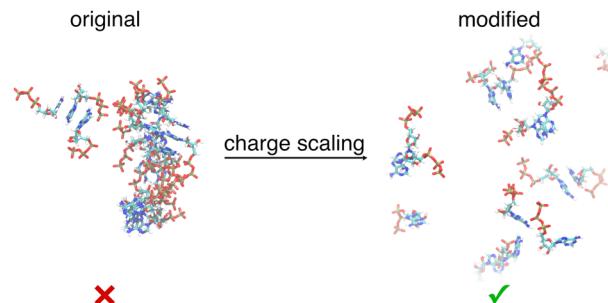
Davide Zeppilli and Laura Orian\*



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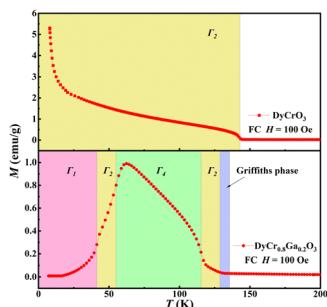
**Development of a force field for ATP – how charge scaling controls self-association**

Tuan Minh Do,\* Nobuyuki Matubayasi and Dominik Horinek\*

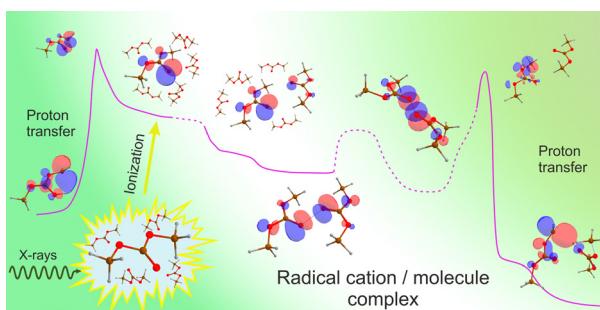


## RESEARCH PAPERS

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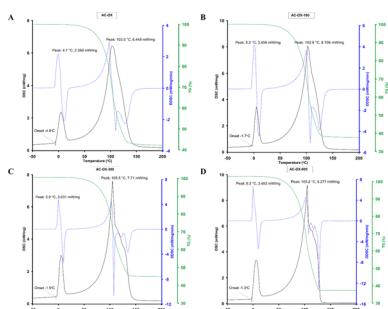
**Multiple spin reorientation transitions in  $\text{Ga}^{3+}$ -substituted  $\text{DyCrO}_3$** Xiong-Han Liu, Meng-Qi Ye, Hai-Bo Xiao,\*  
Shi-Heng Liang, Zheng-Cai Xia and Rui-Long Wang\*

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**Primary radical ions in irradiated carbonates**

Irina S. Tretyakova and Vsevolod I. Borovkov\*

6356

**The influence of surface chemistry of activated carbons on adsorption and freezing/melting processes**Alicja Bosacka,\* Małgorzata Zienkiewicz-Strzałka,  
Anna Deryło-Marczewska,\* Agnieszka Chrzanowska,  
Małgorzata Wasilewska and Piotr Pięta

## CORRECTION

6372

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

Lazaros Chalkopiadis, Konstantinos Lambropoulos and Constantinos Simserides\*