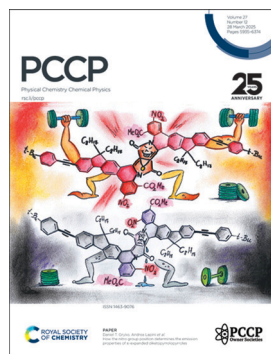


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ISSN 1463–9076 CODEN PPCPFQ 27(12) 5935–6374 (2025)



### 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.

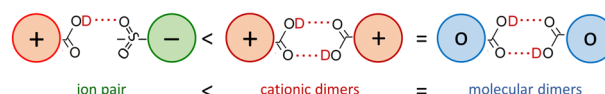
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Alexander E. Khudozhitkov, Lasse Hunger, Loai Al-Sheakh, Alexander G. Stepanov, Daniil I. Kolokolov\* and Ralf Ludwig\*

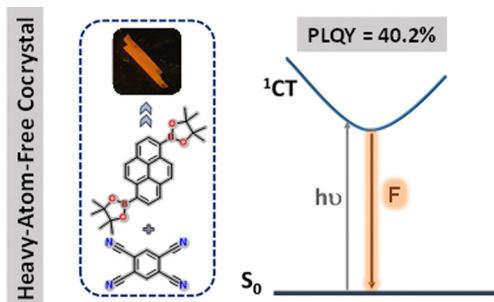
#### Curious Hydrogen Bond Strength



5956

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

Suvarna Sujilkumar and Mahesh Hariharan\*



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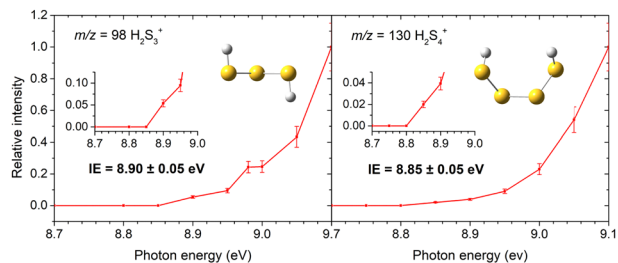
**SAVE  
10%**



5961

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

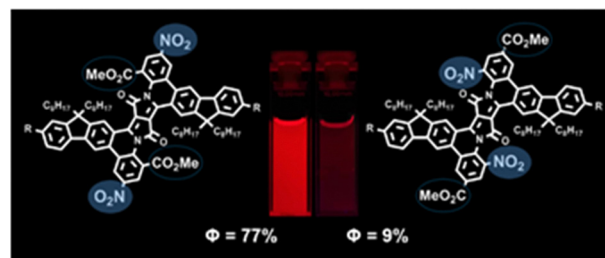
Zhibiao Li, Jianchao Yang, Xinyue Gong, Weijun Zheng, Chongqin Zhu\* and Cheng Zhu\*



5965

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

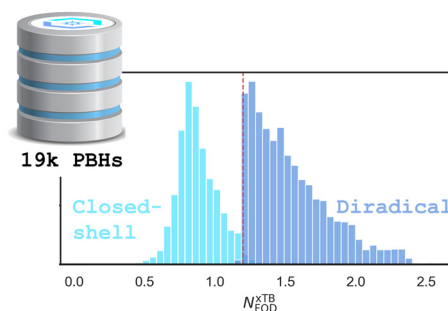
Kamil Skonieczny, Francesco Di Maiolo, Sara Venturi, Alessandro Iagatti, Alessandro Ricci, Francesco Bertocchi, Daniel T. Gryko\* and Andrea Lapini\*



5973

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

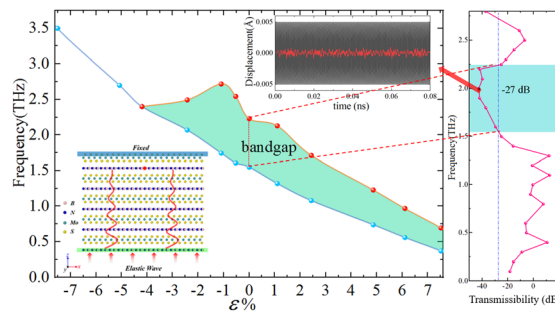
Alexandra Wahab and Renana Gershoni-Poranne\*



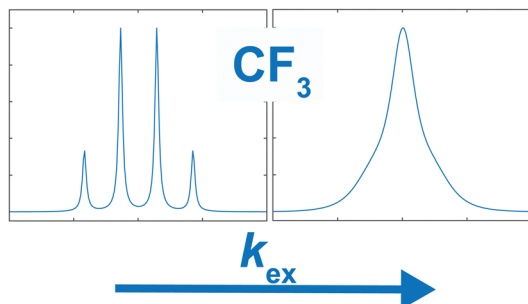
5984

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

Yabin Jing, Lifeng Wang\* and Eric Li



5995

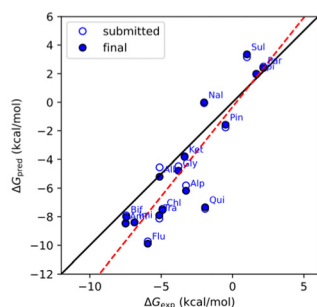
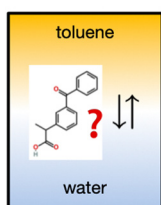


### The influence of fluorine spin-diffusion on $^{13}\text{C}$ solid-state NMR line shapes of $\text{CF}_3$ groups

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

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SAMPL9 logP challenge

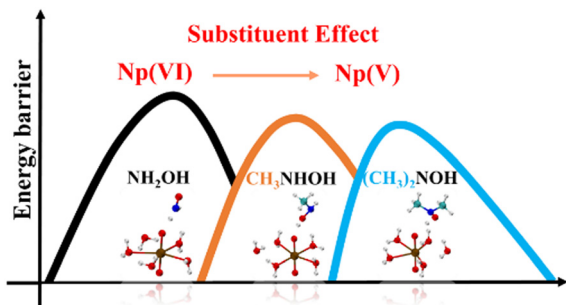


Expanded Ensemble (EE) MD + OpenFF 2.0.0

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

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

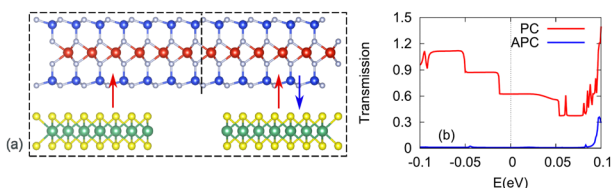
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### Theoretical study on the kinetic behavior of $\text{Np}(\text{VI})$ reduction by hydroxylamine and its derivatives: substituent effect

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

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### 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

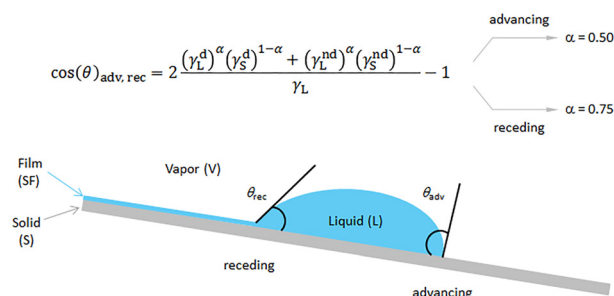


## RESEARCH PAPERS

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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

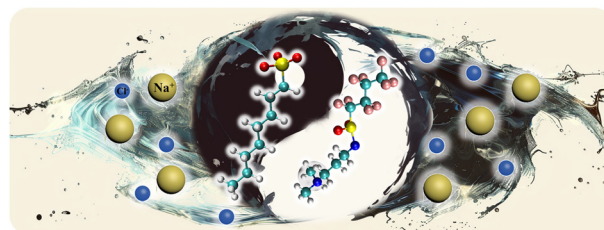
Aliakbar Roosta,\* Sohrab Zendeboudi and Nima Rezaei



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

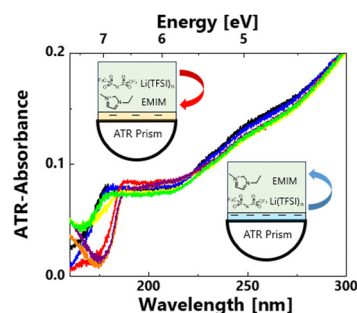
Xiaolong Quan, Jing Xiong, Tong Tong, Jinqing Jiao,\* Jianping Zou and Yuechang Wei\*



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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

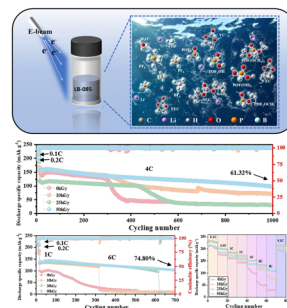
Tomonori Kakinoki,\* Akihito Imanishi, Shinji Kondou, Ichiro Tanabe and Ken-ichi Fukui\*



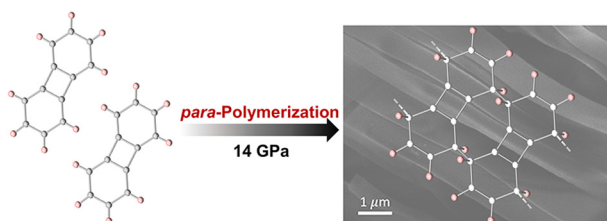
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### High energy electron beam irradiation on the electrolyte enables fast-charging of lithium metal batteries with long-term cycling stability

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



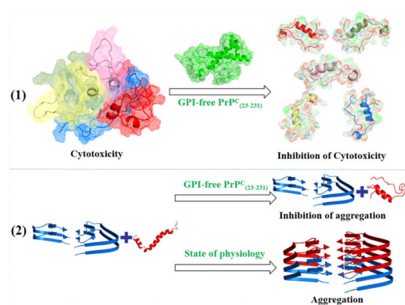
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### Synthesis of a biphenylene nanoribbon by compressing biphenylene under extreme conditions

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\*

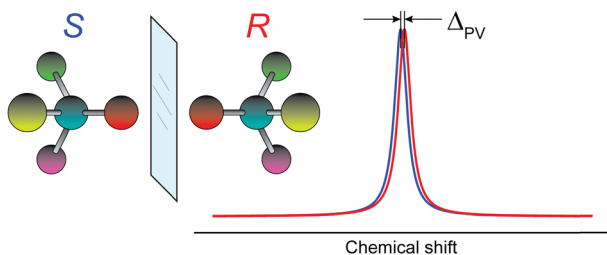
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### Deciphering the full-length PrP<sup>C</sup><sub>(23–231)</sub> receptor and characterizing the size/subphase-dependent impact of Aβ oligomers on the PrP<sup>C</sup><sub>(23–231)</sub> receptor: insights from molecular dynamics simulations

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

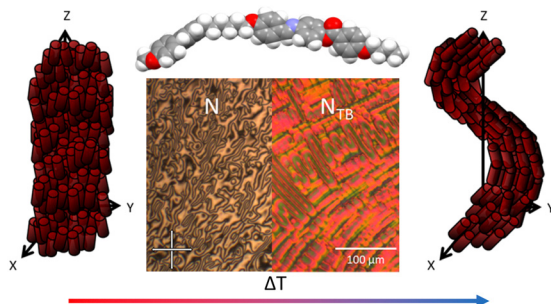
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### Towards detection of molecular parity violation via chiral co-sensing: the <sup>1</sup>H/<sup>31</sup>P model system

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\*

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

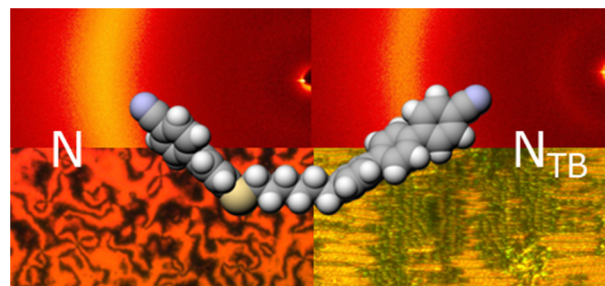
Calum J. Gibb,\* Magdalena M. Majewska, Grant J. Strachan, Damian Pocięcha, John M. D. Storey,\* Ewa Gorecka and Corrie T. Imrie



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

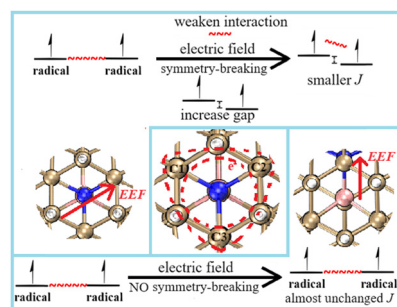
Ewan Cruickshank,\* Grant J. Strachan, Abigail Pearson, Damian Pocięcha, Ewa Gorecka, John M. D. Storey and Corrie T. Imrie



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

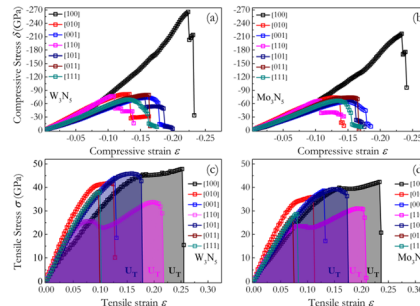
Zhuxiao Li, Zhiru Zhang, Yuxiang Bu and Xinyu Song\*



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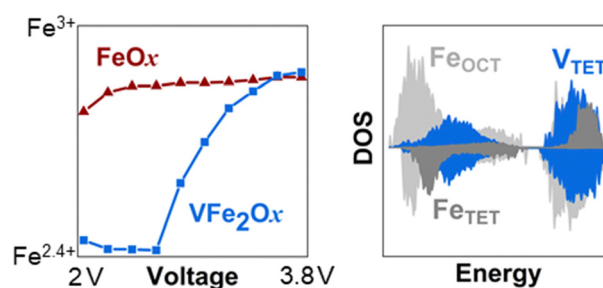
Haiyan Yan, Wenhui Zhang, Lei Chen, Yun Zhang, Hui Wang, Meiguang Zhang\* and Qun Wei\*



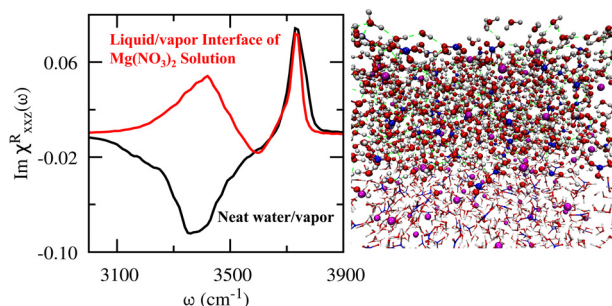
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### Deconvolving lithium-ion redox in vanadium–iron oxide aerogels using X-ray absorption spectroscopy and density functional theory

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



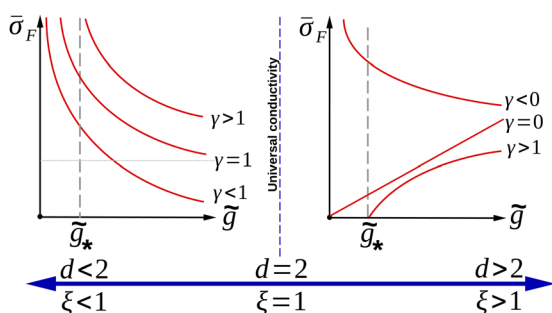
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Effects of cations on the structure, dynamics and vibrational sum frequency generation spectroscopy of liquid/vapor interfaces of aqueous solutions of monovalent and divalent metal nitrates

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

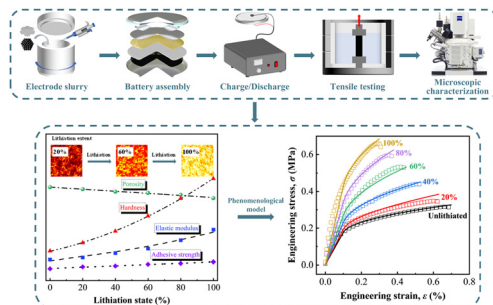
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Disorder driven peculiarities of metal-insulator transition in the interacting fermions ensemble

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

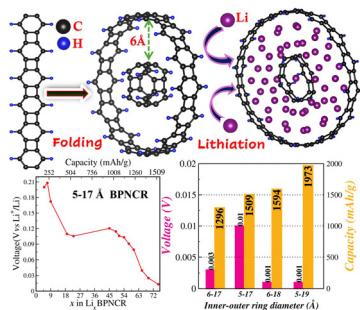
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Revealing the mechanical behaviour and material micro-structure of graphite electrode coatings in lithium-ion batteries during lithiation

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\*

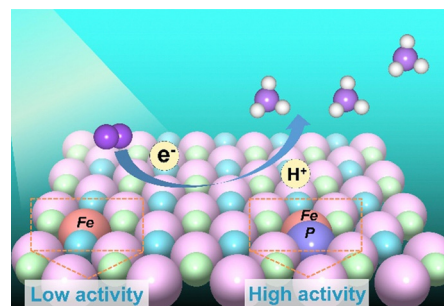


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### Regulating the spin state of a single Fe atom in BiOBr to enhance photocatalytic nitrogen reduction: insights from theoretical studies

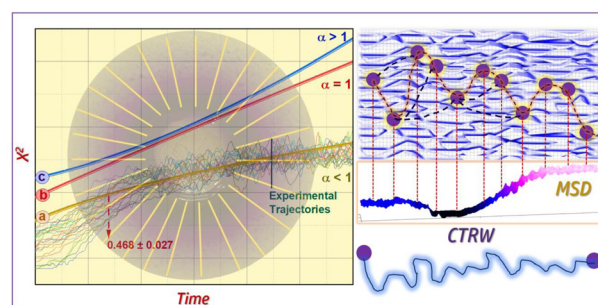
Zhanjin Wang, Xiao Han and Jinlu He\*



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

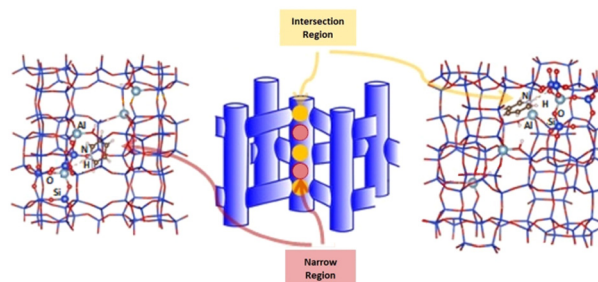
Rachana D. Bamb, Prasad C. Walimbe, Sunil D. Kulkarni\* and Preeti S. Kulkarni\*



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

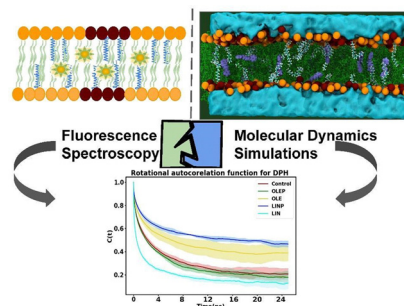
E. Kassab\* and M. Castellà-Ventura



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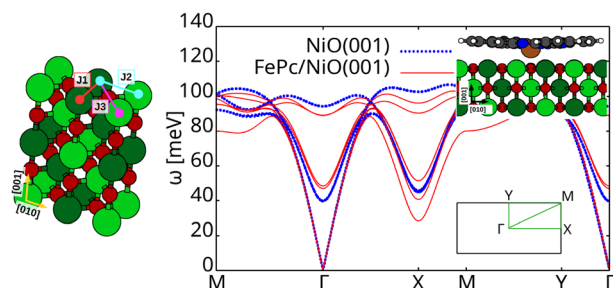
### Anomalous membrane organization by omega-6 and omega-9 fatty acids

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



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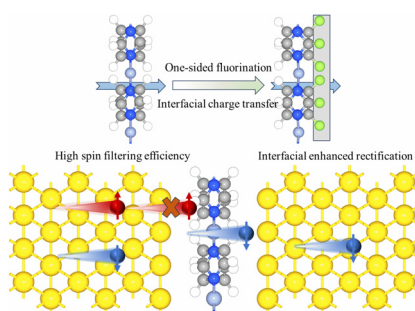
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### Chemical tuning of magnons in NiO(001) by Fe-phthalocyanine adsorption

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

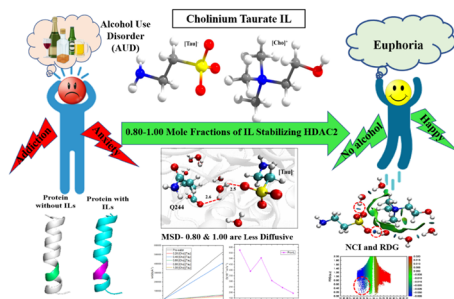
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### Interface-driven spin filtering and diode effects in van der Waals junctions based on magnetic metal–organic frameworks

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

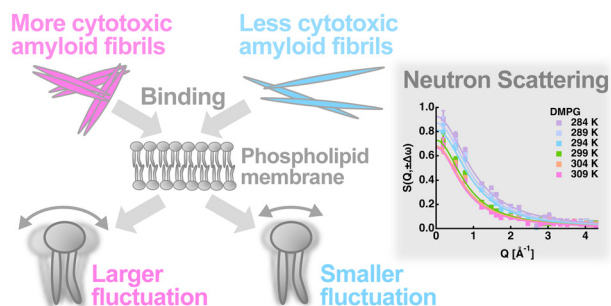
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### Molecular mechanism behind the cholinium-taurate ionic liquid in stabilisation of HDAC2 for alcohol use disorders: insights from DFT and MD simulations

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

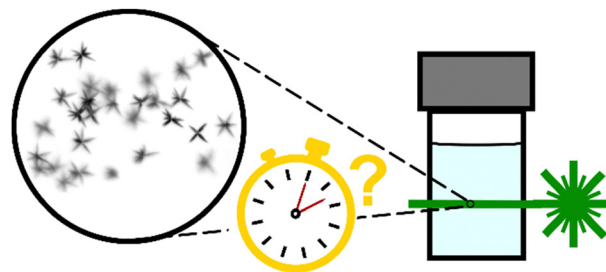
Tatsuhito Matsuo,\* Agathe Bélimé, Francesca Natali, Alessio De Francesco and Judith Peters\*



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

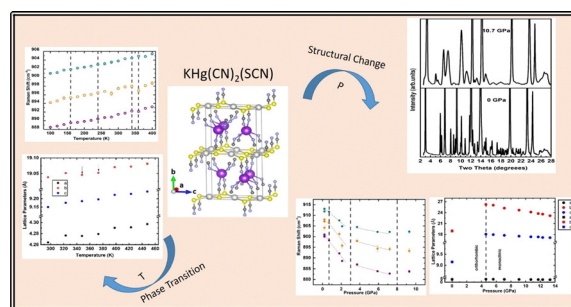
Eleanor R. Barber and Andrew J. Alexander\*



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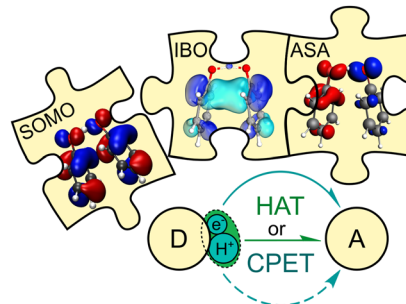
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### Concerted proton electron transfer or hydrogen atom transfer? an unequivocal strategy to discriminate these mechanisms in model systems

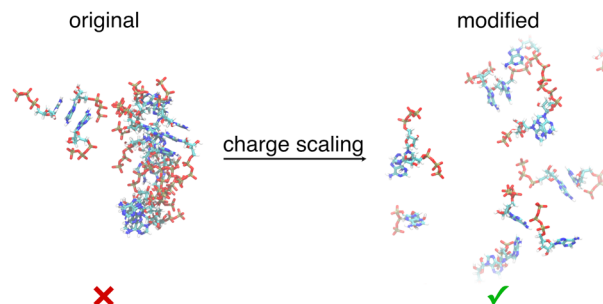
Davide Zeppilli and Laura Orian\*



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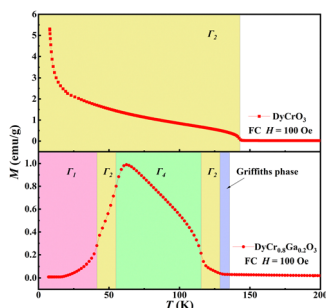
### Development of a force field for ATP – how charge scaling controls self-association

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



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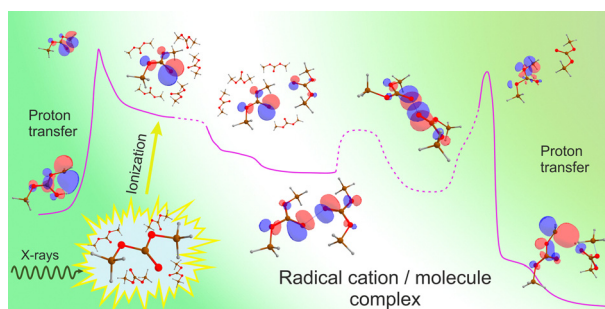
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### Multiple spin reorientation transitions in $\text{Ga}^{3+}$ -substituted $\text{DyCrO}_3$

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

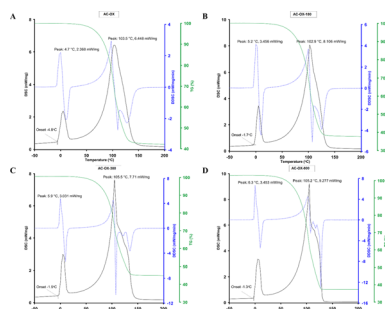
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Irina S. Tretyakova and Vsevolod I. Borovkov\*

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Anna Deryto-Marczewska,\* Agnieszka Chrzanowska,  
Małgorzata Wasilewska and Piotr Pikuta

## CORRECTION

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Lazaros Chalkopiadis, Konstantinos Lambropoulos and Constantinos Simserides\*

