

## IN THIS ISSUE

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### Cover

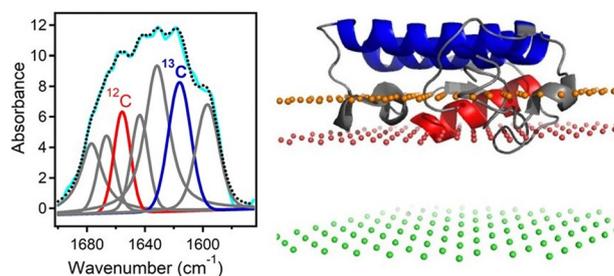
See Hannu Häkkinen *et al.*, pp. 21954–21964. Image reproduced by permission of Maryam Sabooni Asre Hazer from *Phys. Chem. Chem. Phys.*, 2024, 26, 21954.

## TUTORIAL REVIEW

21930

### Analysis of protein–protein and protein–membrane interactions by isotope-edited infrared spectroscopy

Suren A. Tatulian

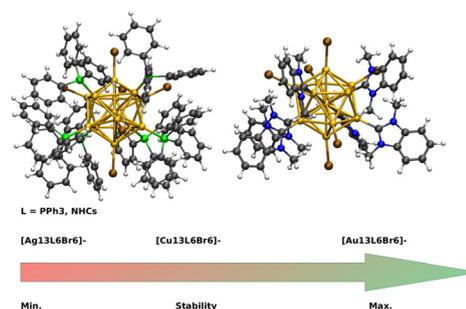


## RESEARCH PAPERS

21954

### Metal–ligand bond in group-11 complexes and nanoclusters

Maryam Sabooni Asre Hazer, Sami Malola and Hannu Häkkinen\*



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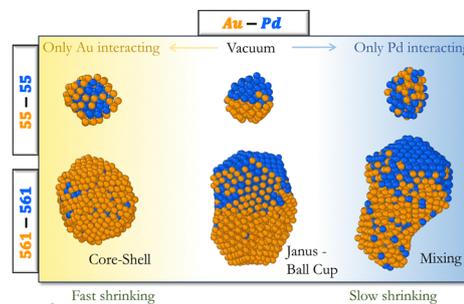
[rsc.li/professional-development](https://rsc.li/professional-development)



21965

### Coalescence of AuPd nanoalloys in implicit environments

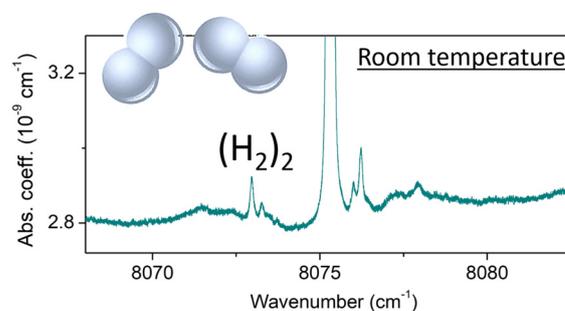
Sofia Zinzani and Francesca Baletto\*



21974

### Room temperature detection of the $(\text{H}_2)_2$ dimer

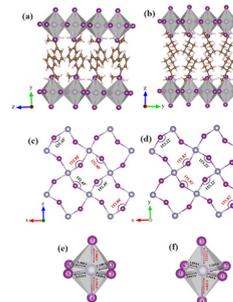
H. Fleurbaey, S. Kassi and A. Campargue\*



21982

### Unraveling the influence of organic cations on tuning electronic structures and spin-splitting in two-dimensional layered organic-inorganic tin-iodine perovskites

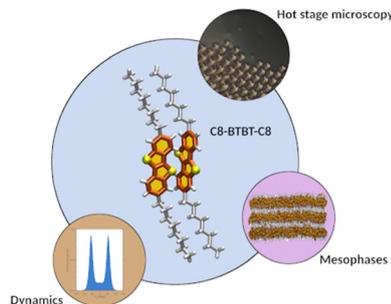
Abdesslem Jedidi,\* Shatha M. Alamri, Norah O. Alotaibi, Souraya Goumri-Said\* and Mohammed Benali Kanoun\*



21990

### Exploring the phase behavior of C8-BTBT-C8 at ambient and high temperatures: insights and challenges from molecular dynamics simulations

Mosè Casalegno,\* Simone Provenzano, Guido Raos and Massimo Moret\*

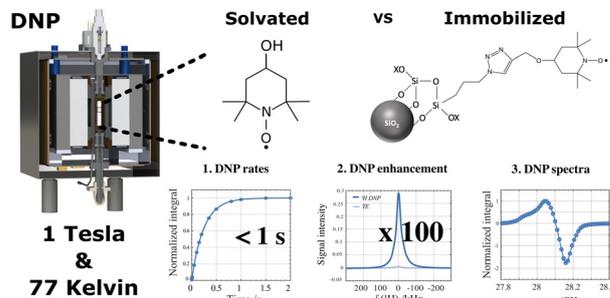




22049

### Full optimization of dynamic nuclear polarization on a 1 tesla benchtop polarizer with hyperpolarizing solids

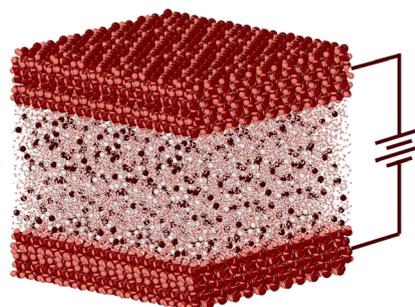
Ewoud Vaneekhaute,\* Charlotte Bocquelet, Léa Bellier, Huu-Nghia Le, Nathan Rougier, Shebha Anandhi Jegadeesan, Sanjay Vinod-Kumar, Guinevere Mathies, Laurent Veyre, Chloe Thieuleux, Roberto Melzi, Daniel Banks, James Kempf, Quentin Stern and Sami Jannin



22062

### Water and ions in electrified silica nano-pores: a molecular dynamics study

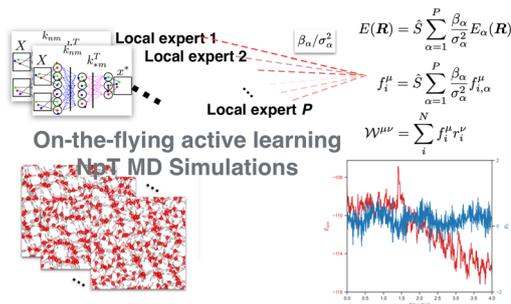
Mahdi Tavakol\* and Kislou Voitchovsky\*



22073

### Active sparse Bayesian committee machine potential for isothermal–isobaric molecular dynamics simulations

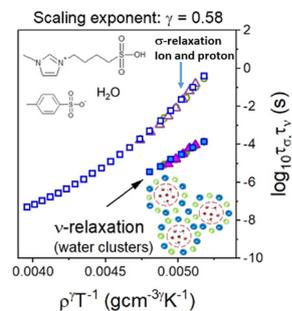
Soohaeng Yoo Willow, Dong Geon Kim, R. Sundheep, Amir Hajibabaei, Kwang S. Kim and Chang Woo Myung\*



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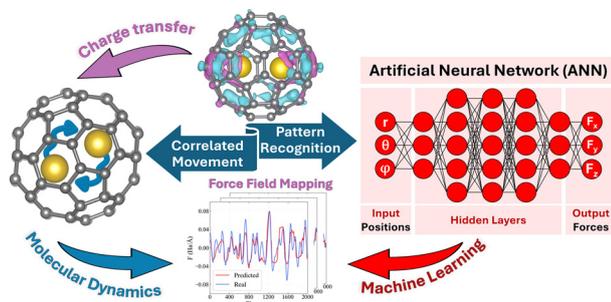
### Origin of $\rho^{\gamma}/T$ scaling of primary and secondary conductivity relaxation times in mixture of water with protic ionic liquid

K. L. Ngai



## RESEARCH PAPERS

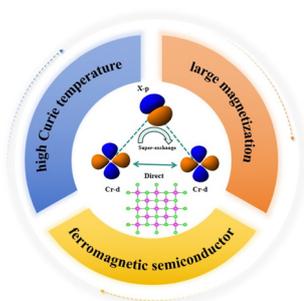
22090



### Collective dynamics of Ca atoms encapsulated in C<sub>60</sub> endohedral fullerenes

Mihaela Cosinschi, Amanda T. Preda, C.-A. Pantis-Simut, N. Filipoiu, I. Ghitiu, M. A. Dulea, L. Ion, A. Manolescu and G. A. Nemnes\*

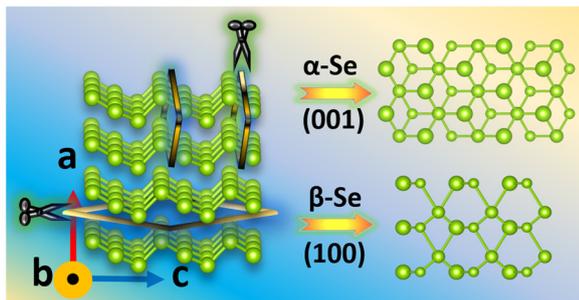
22099



### Two-dimensional ferromagnetic semiconductor Cr<sub>2</sub>XP: first-principles calculations and Monte Carlo simulations

Xiao-Ping Wei,\* Lan-Lan Du, Jiang-Liu Meng and Xiaoma Tao

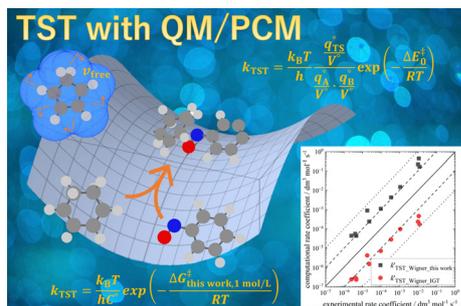
22112



### Multivalency-induced structural variations of 2D selenium nanosheets: facile solution-phase synthesis and optical properties

Swathi V. M., Arjun K., Anju Rajan, Raghu Chatanathodi, Karthikeyan Balasubramanian and Aji A. Anappara\*

22122



### Computation of rate coefficients in solutions based on transition state theory combined with a heuristically corrected polarizable continuum model: intermolecular Diels–Alder reactions as case studies

Yu-ichiro Izato,\* Mitsuo Koshi and Atsumi Miyake

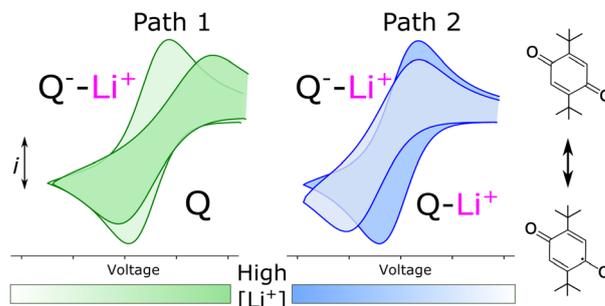


## RESEARCH PAPERS

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### The effect of ionic association on the electrochemistry of redox mediators for Li–O<sub>2</sub> batteries: developing a theoretical framework

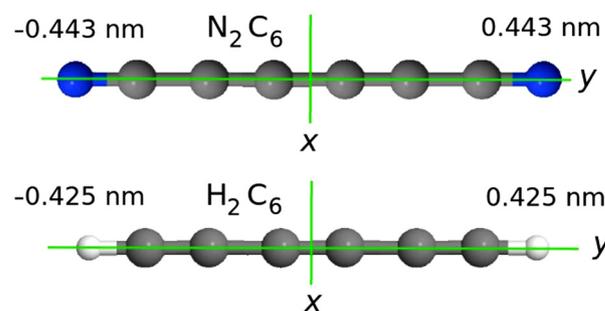
Gabriela Horwitz, Vera Kunz, Samuel P. Niblett and Clare P. Grey\*



22149

### Electronic structure, absorption spectra and oxidation dynamics in polyynes and dicyanopolyynes

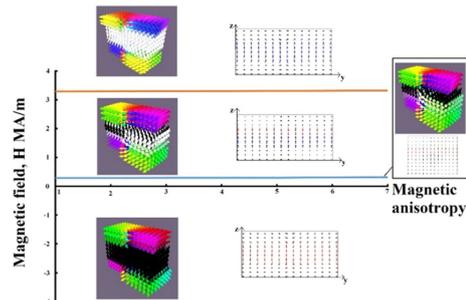
Lazaros Chalkopiadis, Konstantinos Lambropoulos and Constantinos Simserides\*



22164

### Magnetolectric effects in magnetic films with alternating magnetic anisotropy: the emergence and stability of Bloch points

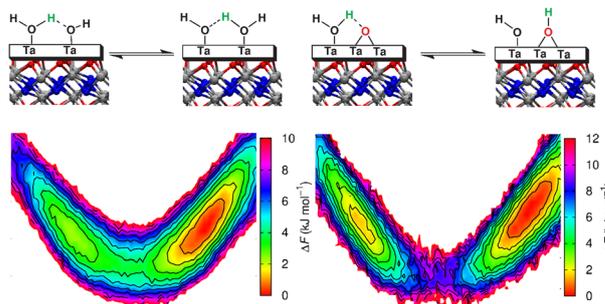
Zukhra Gareeva,\* Viktoria Filippova, Nikolai Shulga and Rurik Doroshenko



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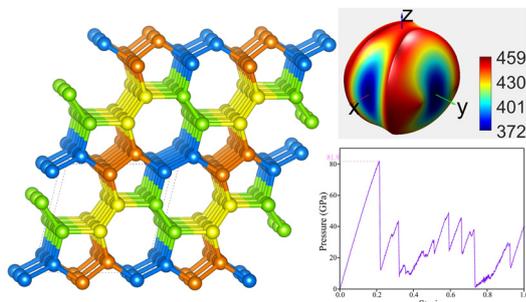
### Molecular insights into the water dissociation and proton dynamics at the $\beta$ -TaON (100)/water interface

Sagarmoy Mandal and Tushar Kanti Ghosh\*



## RESEARCH PAPERS

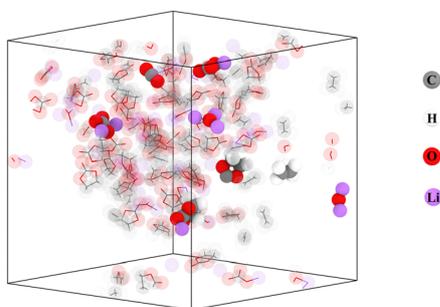
22182



### A novel $sp^3$ carbon allotrope with 4+5+6+7+8 odd-even ring

Tao Yu, Sheng-Cai Zhu\* and Yanglong Hou\*

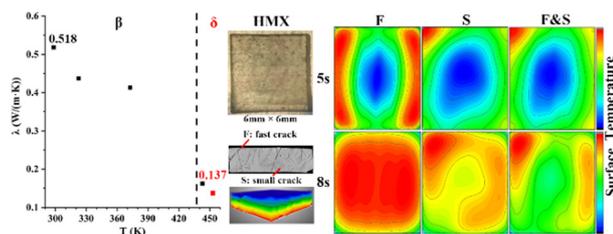
22189



### Comparative study of the reductive decomposition reaction of ethylene carbonate in lithium battery electrolyte: a ReaxFF molecular dynamics study

Jingqi Gao, Ruitian He and Kai H. Luo\*

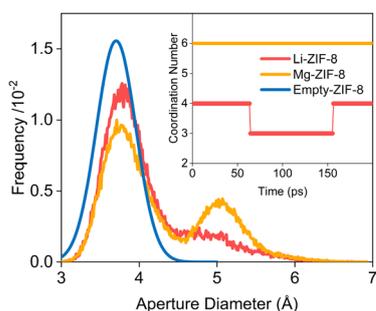
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### Research on the mechanism of threefold discrepancy in thermal conductivity between room temperature and phase transition temperature for 1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) crystals

He Wang, Wentao Liang, Xiangqi Wang, Hao Wang, Di Mai, Cheng Zhong, Xiaoyu Sun, Rucheng Dai, Zhongping Wang, Xianxu Zheng,\* Wanguo Zheng\* and Zengming Zhang\*

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### The mechanisms underlying $Li^+/Mg^{2+}$ separation in ZIF-8 under an electric field from atomistic simulations

Xiang-Long Fu, Fan Zheng, Shi-Jie Xie,\* Yan-Li Ji\* and Cong-Jie Gao

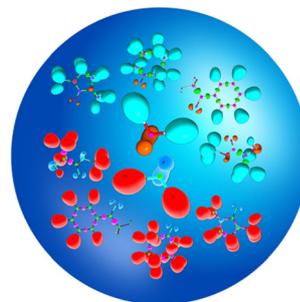


## RESEARCH PAPERS

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**Probing microhydration-induced effects on carbonyl compounds**

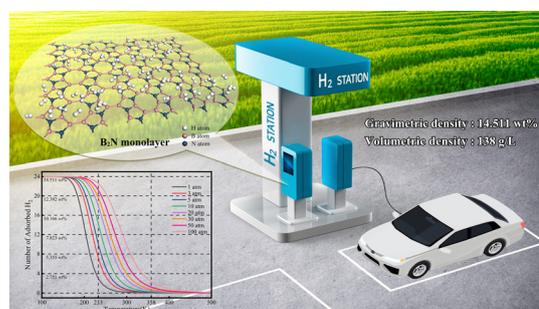
Olivier Aroule, Mahmoud Jarraya, Emilie-Laure Zins\* and Majdi Hochlaf\*



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**Reversible hydrogen storage and release mechanism of a B<sub>2</sub>N monolayer: a first-principles insight**

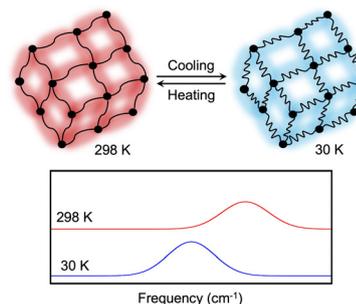
Zonggang Qiu, Jiyuan Guo,\* Qun Wang, Han Wang and Xiangxiang Tan



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**Temperature-dependent structural dynamics in covalent organic frameworks observed by cryogenic infrared spectroscopy**

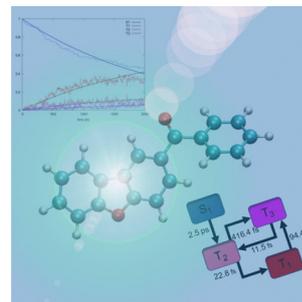
Silas O. Frimpong, Nathan McLane, Matthew Dietrich, Garrison A. Bauer, Michael R. Baptiste, Leah G. Dodson\* and Mercedes K. Taylor\*



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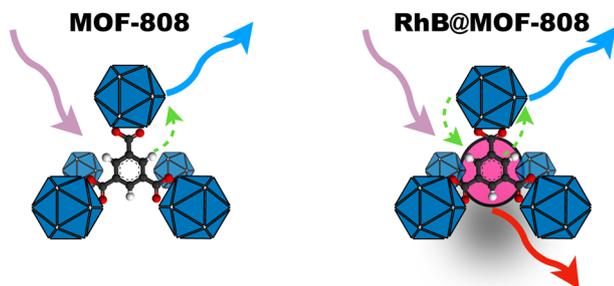
**Intersystem crossing in a dibenzofuran-based room temperature phosphorescent luminophore investigated by non-adiabatic dynamics**

Pelin Ulukan, Elise Lognon,\* Saron Catak and Antonio Monari\*



## RESEARCH PAPERS

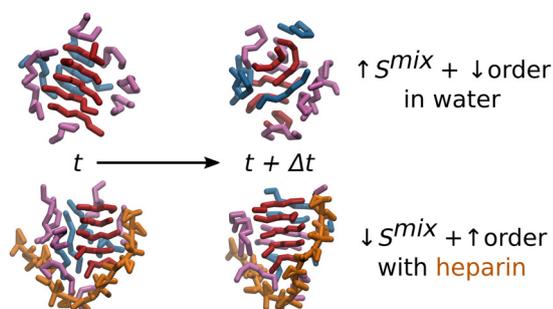
22269



### Unveiling MOF-808 photocycle and its interaction with luminescent guests

G. Ficarra, A. Sciortino,\* L. G. Barbata, R. Ettlinger, V. De Michele, E. Marin, M. Cannas, R. E. Morris and G. Buscarino\*

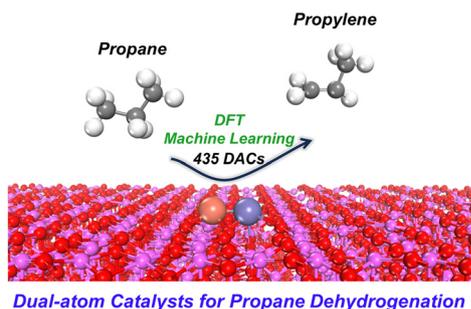
22278



### Unravelling heparin's enhancement of amyloid aggregation in a model peptide system

Suhas Gotla, Anushka Poddar, Ilana Borison and Silvina Matysiak\*

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### Discovery of highly efficient dual-atom catalysts for propane dehydrogenation assisted by machine learning

Xianpeng Wang, Yanxia Ma, Youyong Li, Lu Wang\* and Lifeng Chi\*

## CORRECTIONS

22292

### Correction: First-principles calculations of interfacial thermal transport properties between SiC/Si substrates and compounds of boron with selected group V elements

Zhehao Sun, Kunpeng Yuan, Xiaoliang Zhang\* and Dawei Tang\*



## CORRECTIONS

22293

**Correction: Exploring the properties of  $Zr_2CO_2$ /GaS van der Waals heterostructures for optoelectronic applications**

Altaf Ur Rahman,\* Muhammad Abdul,\* Altaf Karim, Gul Rahman,\* Islam H. El Azab and Bao Jingfu

