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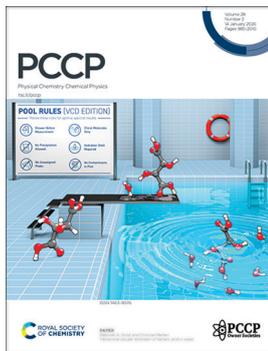
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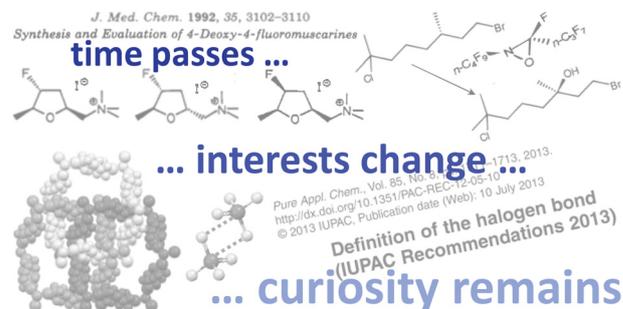
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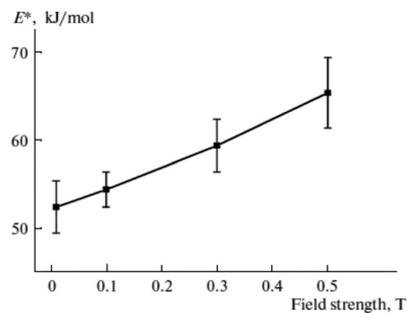


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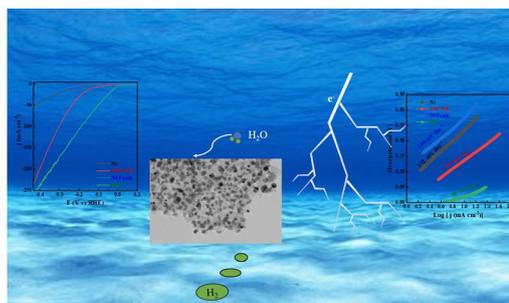
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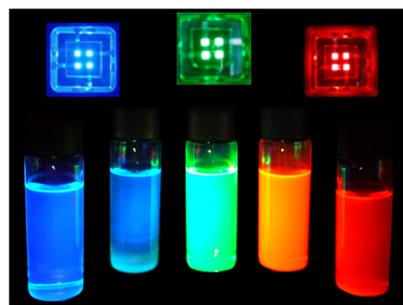


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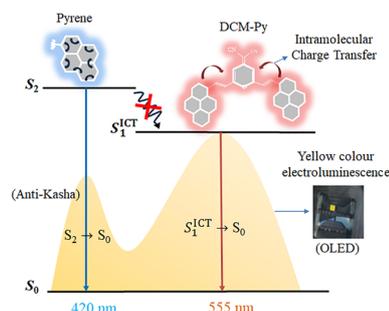


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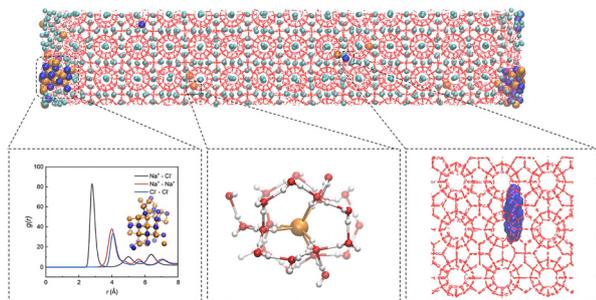
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Abid Ali, Anastasiia S. Kozlenko, Ilya V. Ozhogin, Tomas Vincze, Martin Weis\* and Farman Ali\*



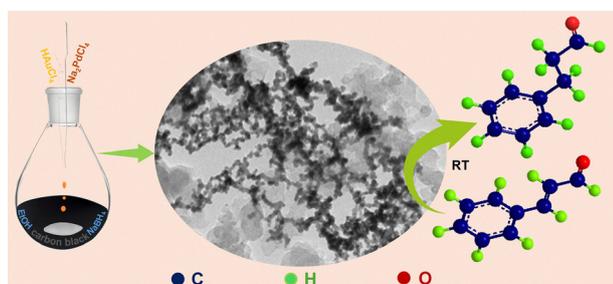
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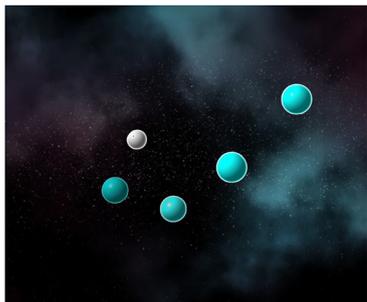
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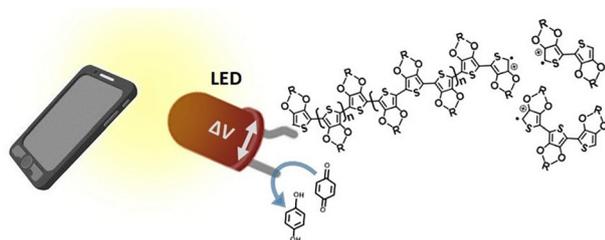
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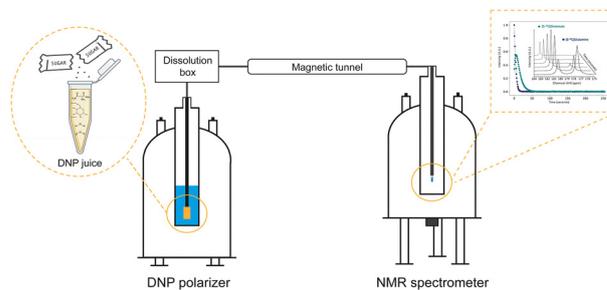


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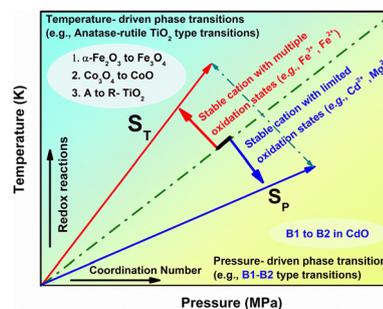
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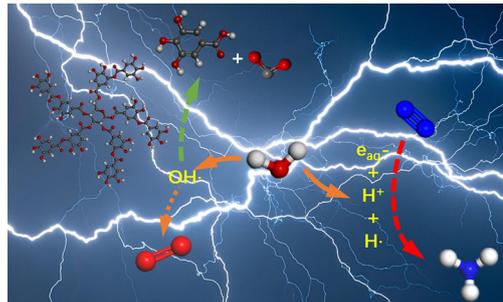
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Jian Liu, Xiao Sun,\* Yang-Yang Zhang, Jun Li\* and Weixin Huang\*

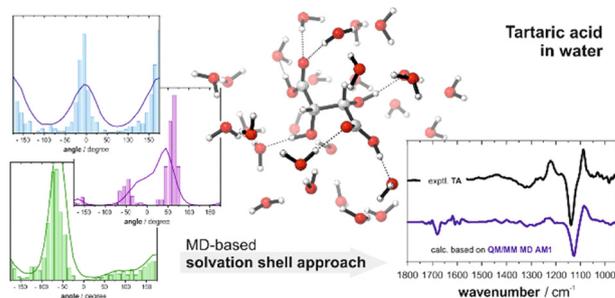


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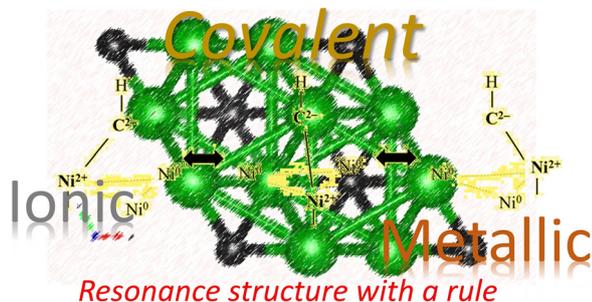
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**Vibrational circular dichroism of tartaric acid in water**

Deborah A. Drost and Christian Merten\*



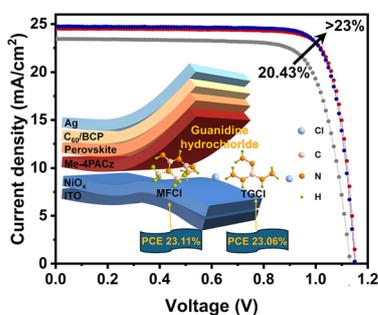
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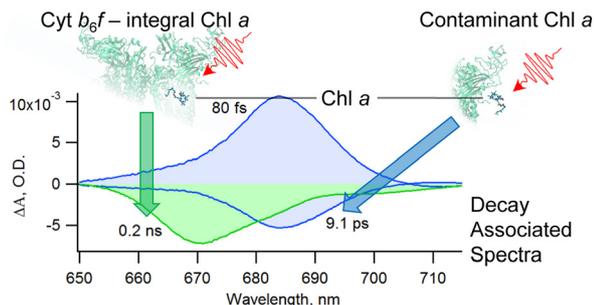
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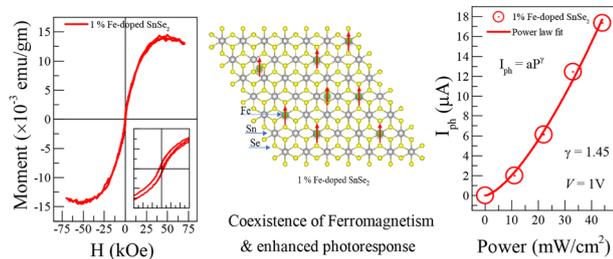
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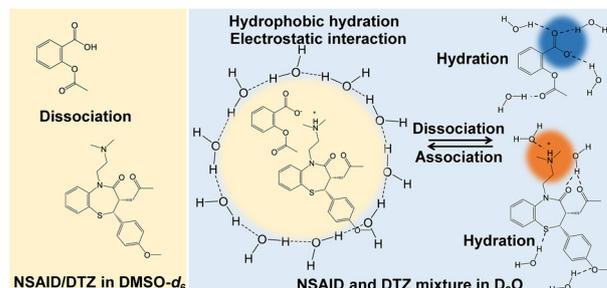


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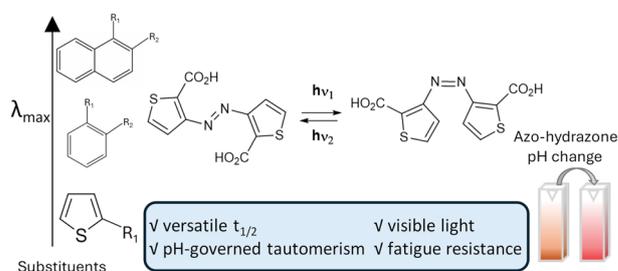
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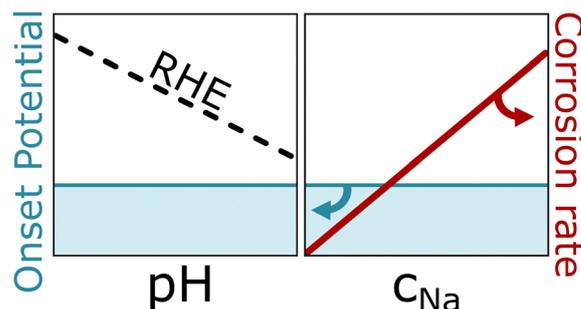
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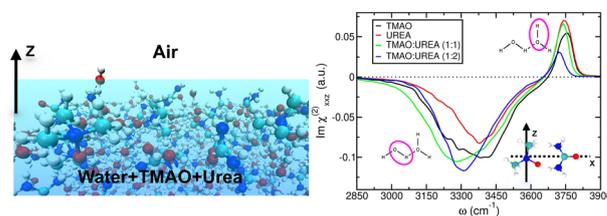
Mark Aarts,\* Jamie A. Trindell and Marc T. M. Koper\*



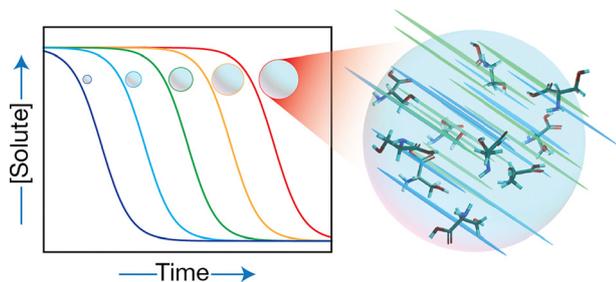
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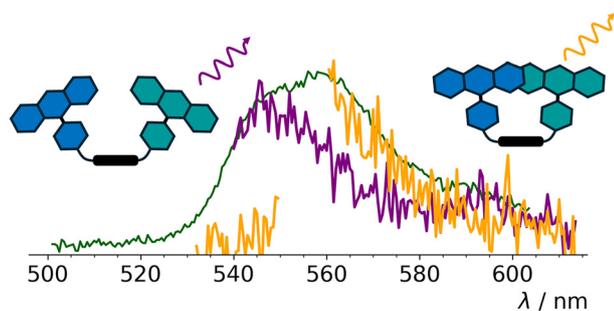
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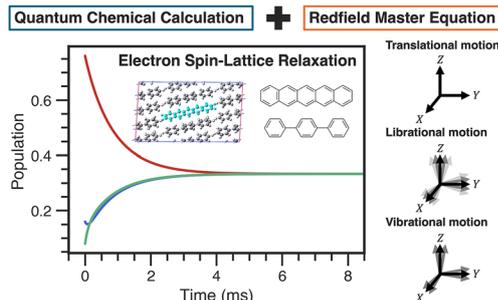
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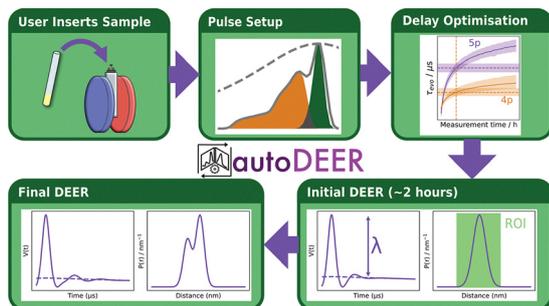
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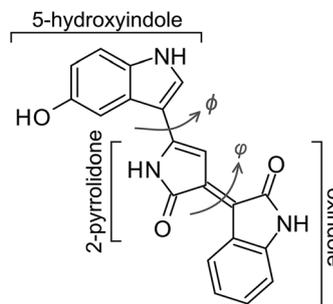


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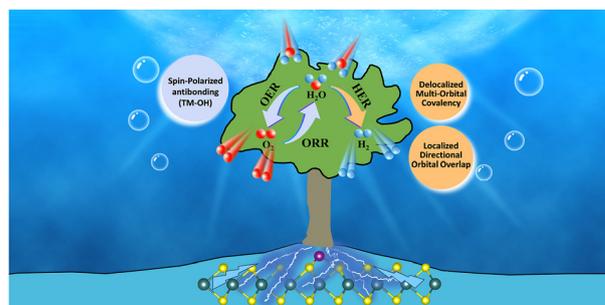
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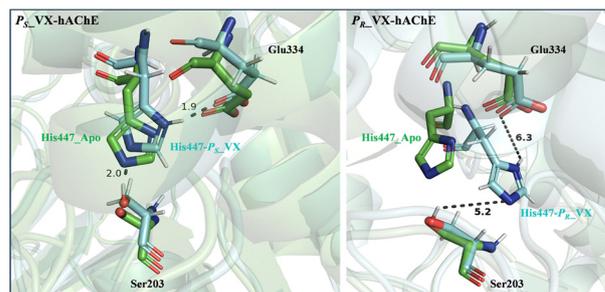
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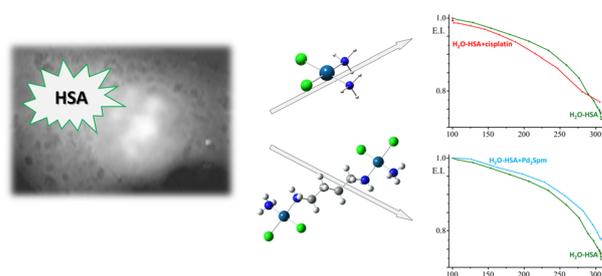
Dipankar Das, Shibaji Ghosh, Kalyanashis Jana and Bishwajit Ganguly\*



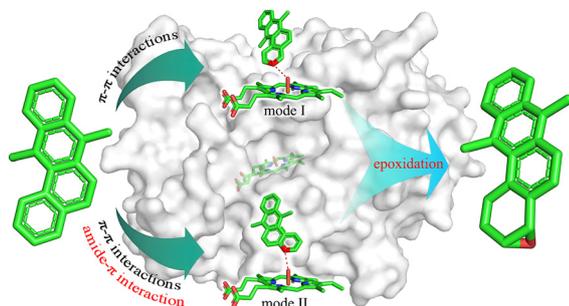
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Clara B. Martins, Mona Sarter, Ana L. M. Batista de Carvalho, Victoria Garcia-Sakai, Tilo Seydel, Jacques Ollivier, Luis A. E. Batista de Carvalho and Maria P. M. Marques\*



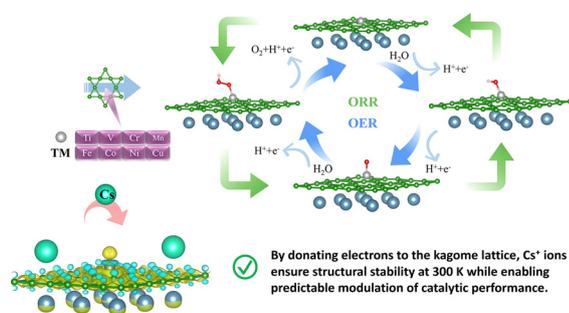
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Chong Liu, Yan Zhao, Shi Feng and Qingchuan Zheng\*

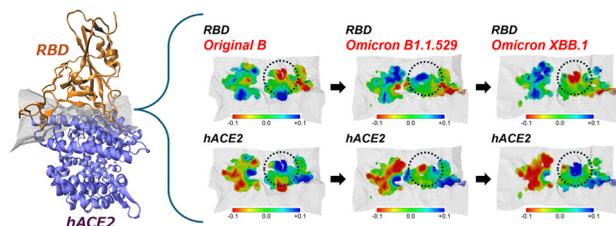
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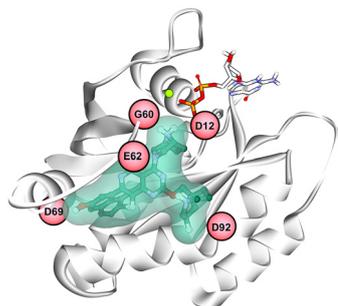
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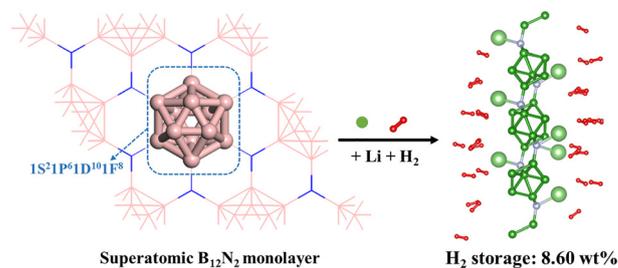


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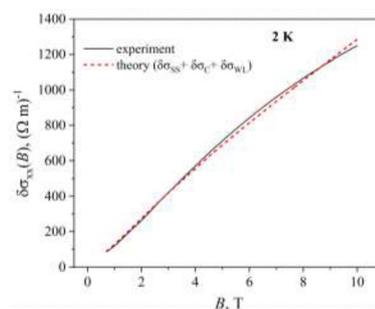
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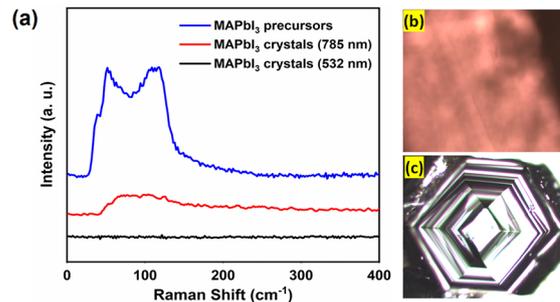
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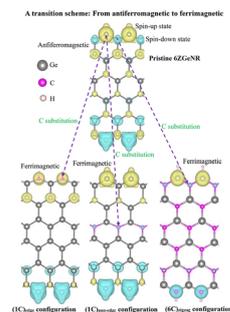
Abdul Zeeshan Khan, Muhammad Shafi, Tarek. A. Kandiel\* and Abdulaziz A. Al-Saadi\*



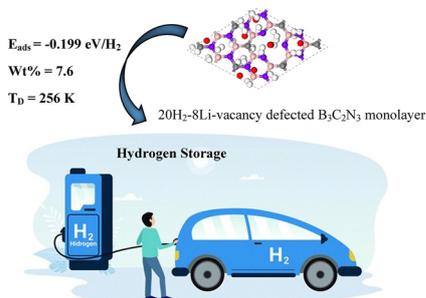
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D. M. Hoat, Ngoc Thanh Thuy Tran, Quoc-Duy Ho, Duc-Quang Hoang, Minh Triet Dang and Duy Khanh Nguyen\*



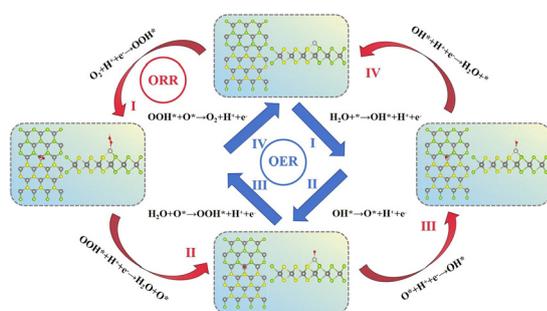
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Kai Zhang, Jianjun Fang, Chenkun Li, Tongmeng Xing, Qiuyan Xiang, Xianfang Yue, Breno R. L. Galvão\* and Jing Li\*

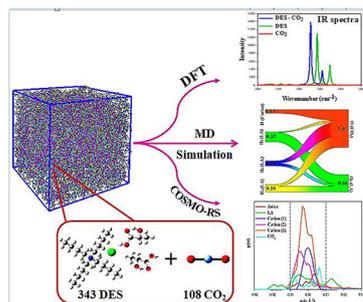
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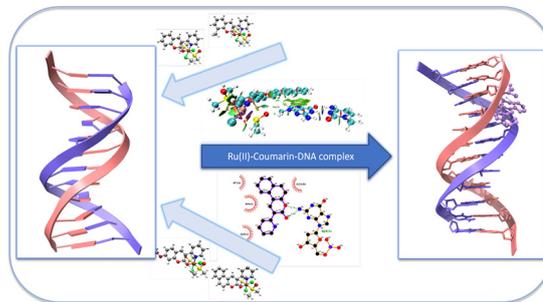


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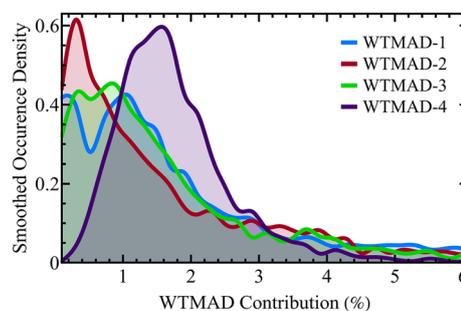
Pratyashee Barukial, Rajib Nandi, Manazira Ahmed, Rituraj Barman, Tamal Banerjee\* and Bipul Bezbaruah\*



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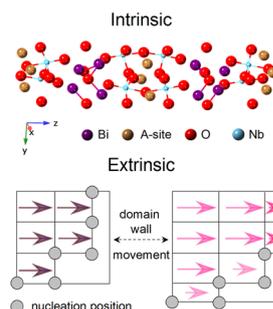
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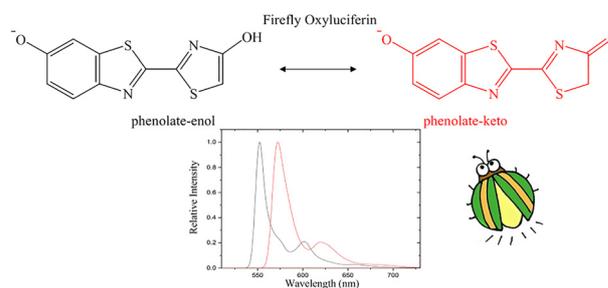
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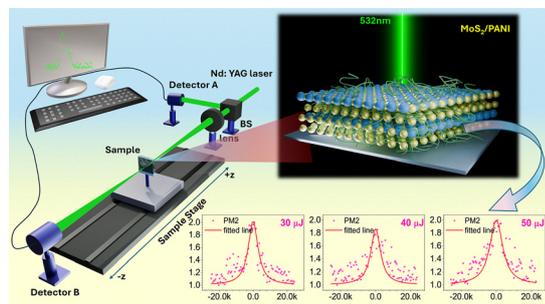
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Shuangqi Pi, Cheng Peng, Haibo Ma\* and Ya-Jun Liu\*



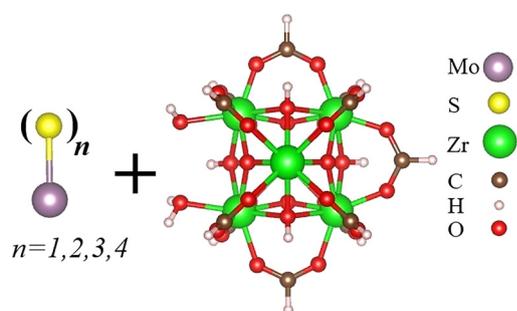
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Anjali Sharma and B. Karthikeyan\*

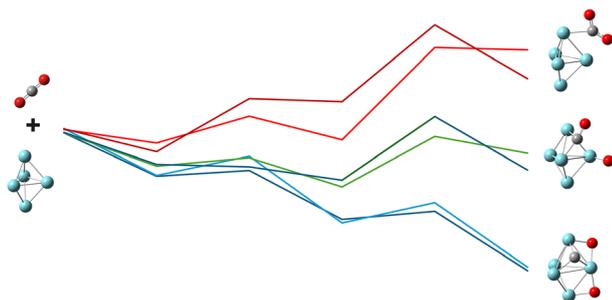
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Maryam Mansoori Kermani, Matthew Neurock and Donald G. Truhlar\*

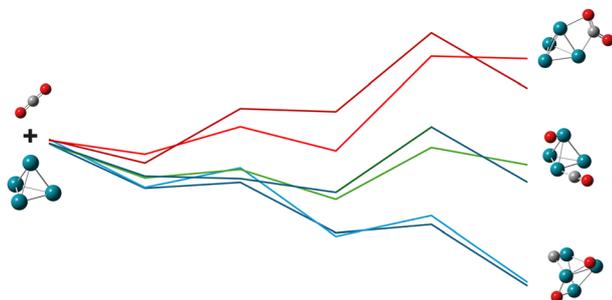
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### Associative vs. dissociative binding of CO<sub>2</sub> on M<sub>5</sub> transition metal clusters

Nguyen T. T. Le, Alireza Nazari, Yash Rele, Mighila Rixon, Ishudeep Singh Narula and Matthew A. Addicoat\*

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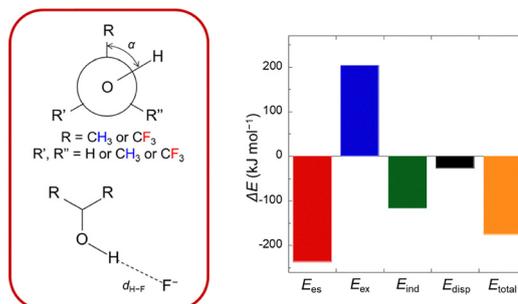
Sherfi Sherif, Bala Aakash Velmurugan, Naeem Abbas, Muskanbanu Shaikh and Matthew A. Addicoat\*



1538

### Effects of the fluorination degree in alcohols on the interaction with fluoride ions

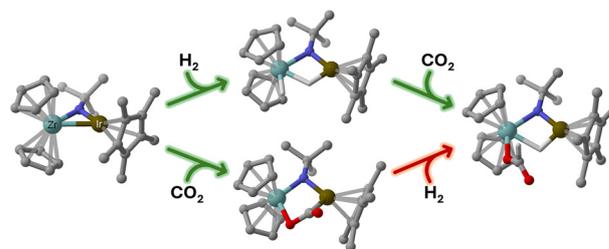
Nozomi Yoneda, Kohei Tada, Seiji Tsuzuki and Kazuhiko Matsumoto\*



1549

### Mechanism, selectivity, and what prevents closure of the catalytic cycle for H<sub>2</sub> reduction of CO<sub>2</sub> promoted by a heterodinuclear zirconium–iridium complex

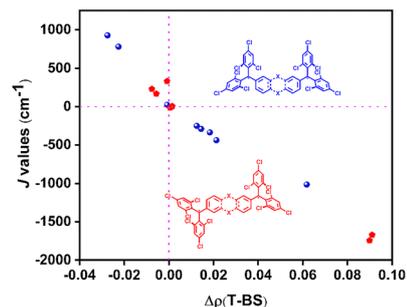
Kevin P. Quirion and Daniel H. Ess\*



1556

### Heteroatom effects on the magnetic exchange interactions in bis(2,4,6-trichlorophenyl)methyl-based diradicals

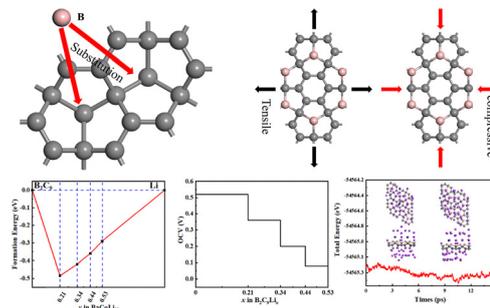
Li Shen,\* Rui Dong, Jia-nan Lang, Yihan Li, Yue Li, Jitao Lu, Qian Wu and Qingguo Meng\*



1565

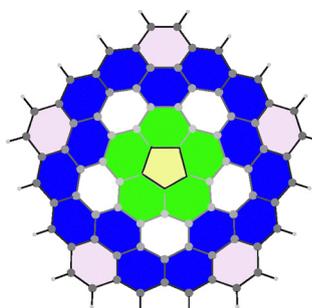
### B<sub>2</sub>C<sub>9</sub> as a high-performance Li-ion battery anode: effects of boron-incorporation and strain-engineering on the adsorption and diffusion of lithium

Rui Shen, Hao Cheng, Guo-Xiang Gao, Xin-Yue Li, Chun-Sheng Liu\* and Xiao-Juan Ye\*



## RESEARCH PAPERS

1573

Carboncane[1,3] ( $C_{80}H_{20}$ )

25 Clar structures with 9 sextets each

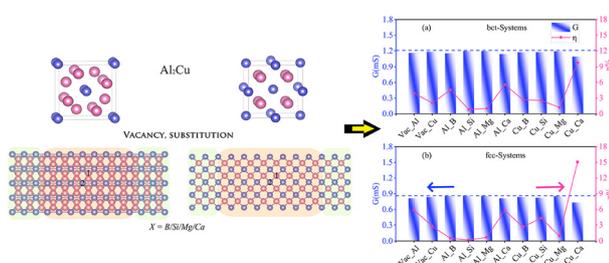
Sextets can be located only in green (6 times) and blue (7 times) rings

A sextet is never found in empty rings

### Paratropic ring currents discovered in six-membered rings of conical nanographenes: carboncones

Francesco F. Summa, Lawrence T. Scott, Riccardo Zanasi\* and Guglielmo Monaco

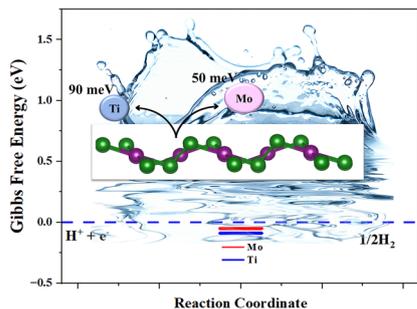
1586



### Impacts of vacancy defects and element substitution on the electrical transport properties of $\theta$ - $Al_2Cu$ and $\delta$ : A NEGF-DFT study

Shumin Yan, Mingyan Chen, Yibin Hu and Yin Wang\*

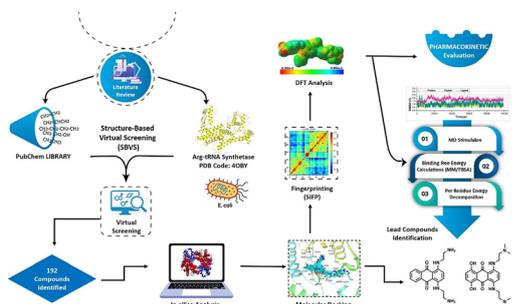
1594



### Unveiling the HER potential of TM-substituted PdTe<sub>2</sub> monolayers: a first-principles study

Poonam Parkar, Ajay Chaudhari\* and Brahmananda Chakraborty\*

1608



### Structure-based virtual screening and MD refinement reveal novel inhibitors of *Escherichia coli* arginyl-tRNA synthetase

M. Bilal Tayyab and Jianshu Dong\*

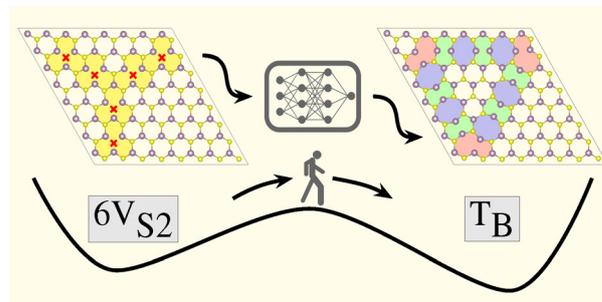


## RESEARCH PAPERS

1626

### Completing the hierarchy of rotational defects in monolayer MoS<sub>2</sub> through symmetry-aware evolutionary search

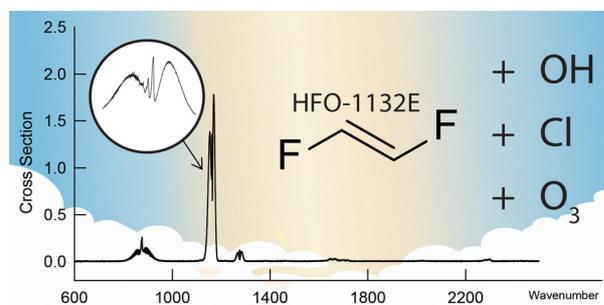
Alexander Adel, Ralf Wanzenböck and Georg K. H. Madsen\*



1634

### Atmospheric chemistry of (*E*)-1,2-difluoroethene: kinetics and mechanisms of the reactions with Cl atoms, OH radicals and O<sub>3</sub>

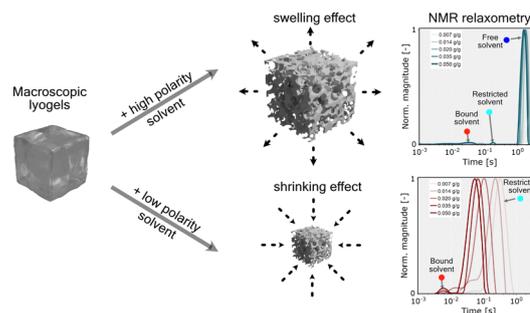
Mads. P. Sulbaek Andersen,\* Ellen R. Kjaergaard, Connor Blair and Ole J. Nielsen



1645

### NMR relaxometry probes solvent-polarity-dependent molecular interactions in stimuli-responsive lyogels

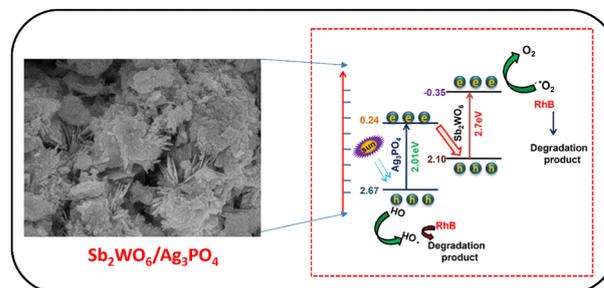
Muhammad Adrian,\* Kathrin Marina Eckert, M. Raquel Serial, Artyom Tsanda, Lukas Rennpferdt, Stefan Benders, Hoc Khiem Trieu, Tobias Knopp, Irina Smirnova and Alexander Penn



1655

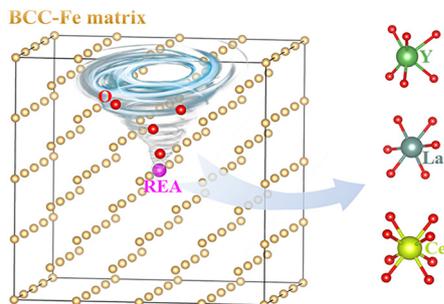
### Development of a novel direct Z-scheme Sb<sub>2</sub>WO<sub>6</sub>/Ag<sub>3</sub>PO<sub>4</sub> nanocomposite with sustainable design for simultaneous electrochemical detection of Pb<sup>2+</sup> and photocatalytic degradation of RhB dye

Nadi Mlihan Alresheedi



## RESEARCH PAPERS

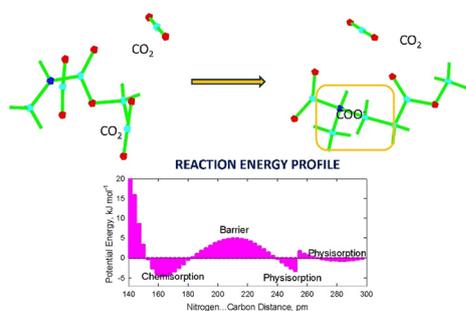
1671



### First-principles investigation of oxygen interstitial solubility, site preference, and nucleation behavior in BCC-Fe doped with rare earth elements (Y, La, Ce)

Liangfu Zhou, Zeyu Wang, Kaiqi Li, Xiaoyang Fu, Rui Ma, Ruixue Tian, Jun Cheng and Lei Ren\*

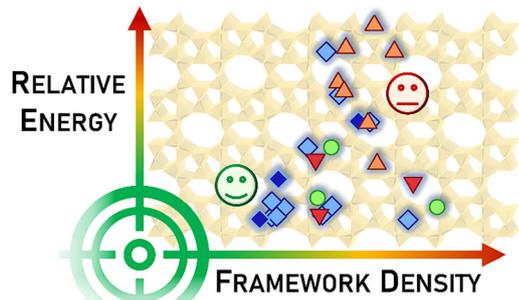
1681



### Investigation of a novel urethane-inspired CO<sub>2</sub> chemisorbent: structure modifications and activation barriers

Vitaly V. Chaban

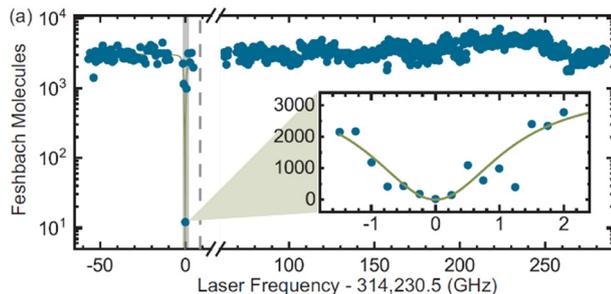
1692



### Balancing accuracy and efficiency in density functional theory studies of SiO<sub>2</sub> polymorphs

Michael Fischer

1705



### Perturbation-assisted observation of the lowest vibrational level of the $b^3\Pi_0$ state of ultracold LiK molecules

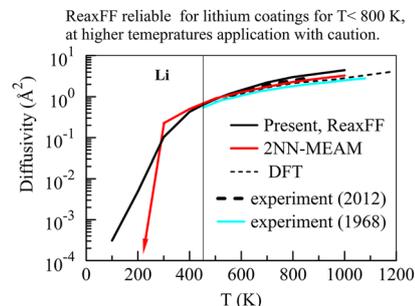
Anbang Yang, Xiaoyu Nie, Hao Lin Yu, Yiming Liu, Victor Avalos, Canming He, Jacek Kłos, Svetlana Kotochigova and Kai Dieckmann\*



1712

### Suitability of the ReaxFF potential for MD modeling of lithium across low and high temperatures

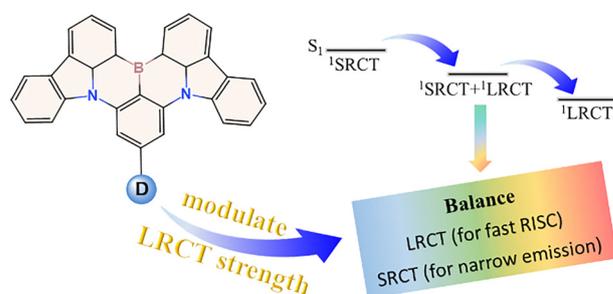
P. S. Krstic,\* S. Dwivedi, A. C. T. van Duin and B. E. Koel



1720

### Modulating excited state via diversified electron-donating units in MR-TADF emitters: a theoretical exploration of structure–property relationships

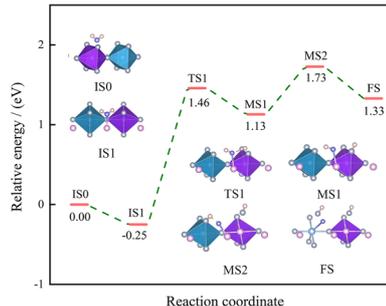
Zhu Chang, Rajat Walia, Dandan Zhang, Xian-Kai Chen and Jiaqi Li\*



1730

### Thermodynamic and kinetic studies of the hydrolysis mechanism of halide solid state electrolytes $\text{Li}_3\text{MCl}_6$ ( $\text{M} = \text{In}, \text{Y}$ )

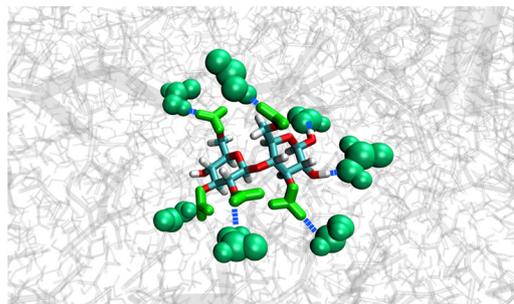
Jian Zhang\* and Shuangtao Pan



1739

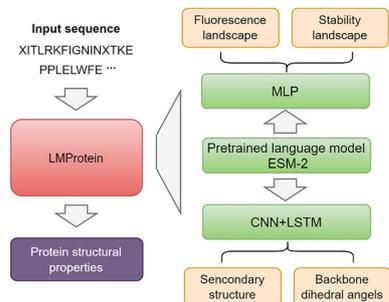
### Molecular origin of high-concentration cellulose dissolution in organic acid media: a combined experimental and computational study

Kanta Hayashi, Tomoya Tashiro, Tomohiro Hashizume, Takashi Watanabe and Kenta Fujii\*



## RESEARCH PAPERS

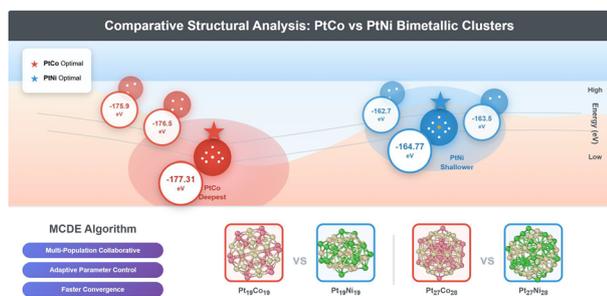
1747



### LMPProtein: a protein language model based framework for protein structural property prediction

Yongna Yuan,\* Hui Luo and Yaojie Tian

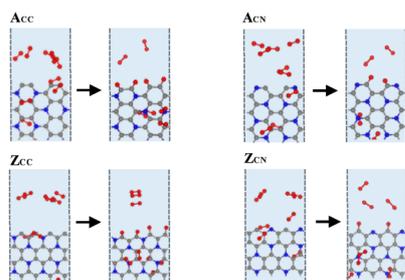
1759



### Comparative structural analysis of PtCo and PtNi bimetallic clusters: a systematic study using the MCDE algorithm

Miao He, Xiaomin Wu,\* Ruoyu Gan, Lin Tao and Yuheng Chen

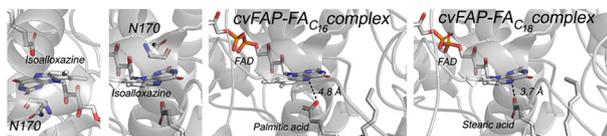
1770

Four types of C<sub>3</sub>N edges can be easily oxidized at O<sub>2</sub> atmospheres.

### Phase diagram and dynamics of the edge oxidation of C<sub>3</sub>N monolayers in O<sub>2</sub> atmosphere from first-principles calculations

Zhongyue Li, Nan Zhao, Haitao Chen\* and Liang Zhao\*

1781



### Effects of substrate length and active-site residue on catalytic function of fatty acid photodecarboxylase

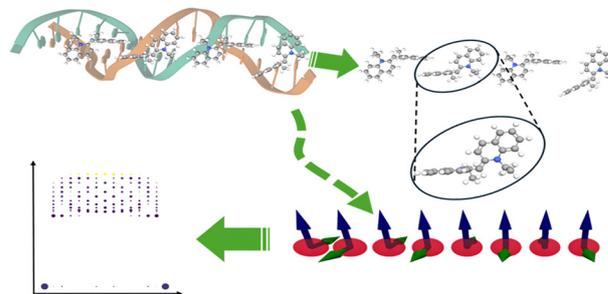
Min-Shih Su and Ya-Ting Kao\*



1792

### Enhancing energy transport utilising permanent molecular dipoles

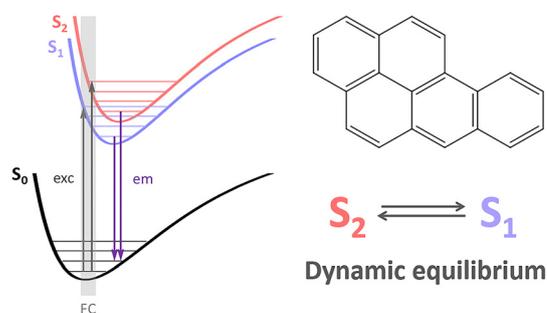
Adam Burgess\* and Erik M. Gauger



1806

### Non-adiabatic quantum dynamics of polycyclic aromatic hydrocarbons exhibiting anti-Kasha emission from the $S_2$ state

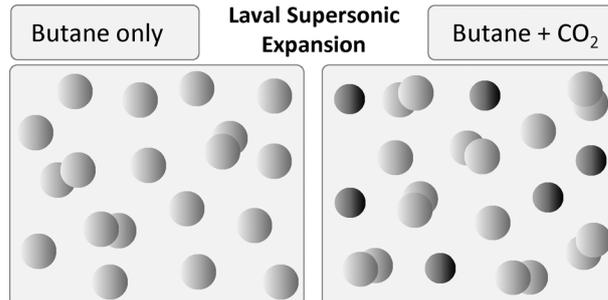
Nikita A. Shekhovtsov\* and Mark B. Bushuev\*



1820

### Acceleration of butane vapor nucleation by carbon dioxide gas

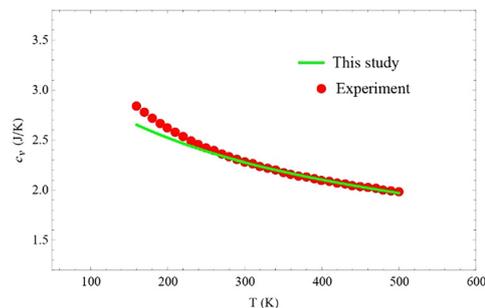
Arnab Choudhury, Felix Graber, Stefan Feusi, Jan Krohn, Jai Khatri, Fernando Torres Hernandez, Chenxi Li and Ruth Signorell\*



1829

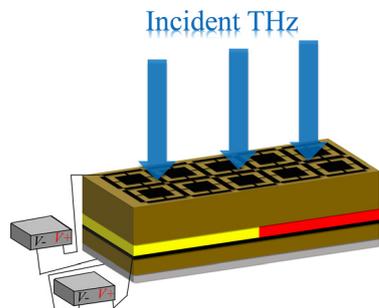
### A study of Frenkel frequency and heat capacity as a function of pressure and temperature using a new approach to the phonon theory of liquids

M. Y. Esmer\* and Bahtiyar A. Mamedov



## RESEARCH PAPERS

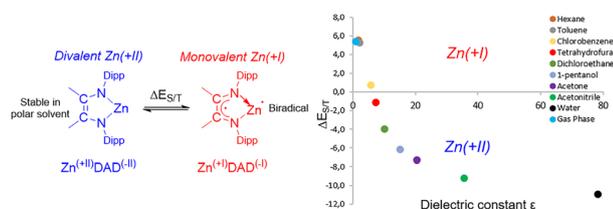
1835



### A switchable and tunable THz metasurface absorber with broadband and dual-band absorption features

Usama Arif, Amna Inayat, Muhammad Mohsin, Muhammad Fasih, Jiang Yue and Wei Su\*

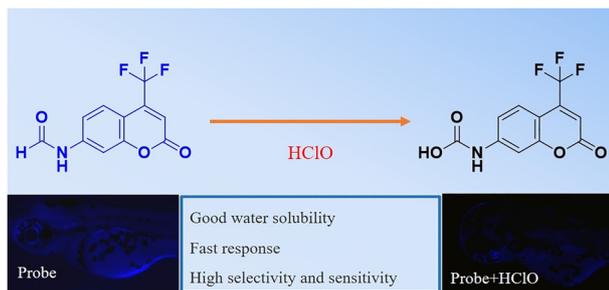
1845



### Solvent-dependent electronic dichotomy in zinc complexes with non-innocent ligands: divalent Zn<sup>(+II)</sup> vs. monovalent Zn<sup>(+I)</sup> forms

Mikaël Le Roch, Alejandro Perez-Luna, H el ene G erard, Fabrice Chemla and St ephanie Halbert\*

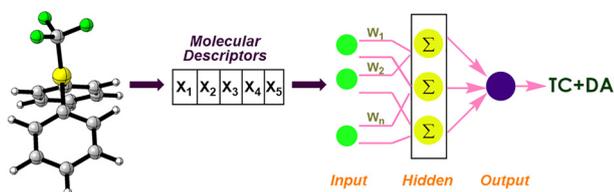
1853



### Development of a novel fluorescent probe for highly sensitive detection and visualization of HClO in environmental and biological systems

Mingshuo Ma, Bingxin Zhu, Shihua Yu, Xiaodan Zeng\* and Zhigang Liu\*

1864



### Interpretable machine learning framework for predicting the reactivity of trifluoromethylating reagents

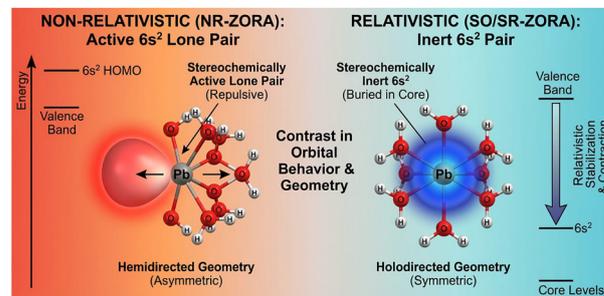
Vaneet Saini\* and Shivansh Kanwar



1877

## Coordination of lead(II) in solvated clusters with water $[\text{Pb}(\text{H}_2\text{O})_{1-8}]^{2+}$ : insights from relativistic effects, energy analysis, molecular orbitals, and electron density

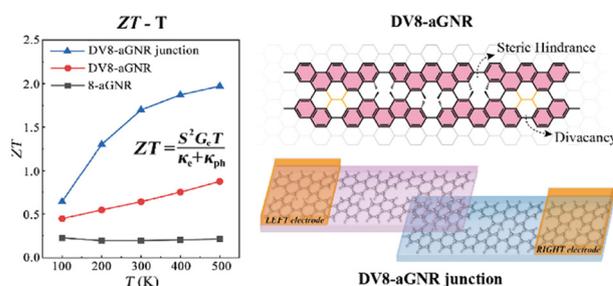
Andy D. Zapata-Escobar,\* Franklin Ferraro, Edison Flórez and Alejandro F. Maldonado\*



1892

## High thermoelectric figure of merit in nonplanar graphene nanoribbons with periodic divacancies

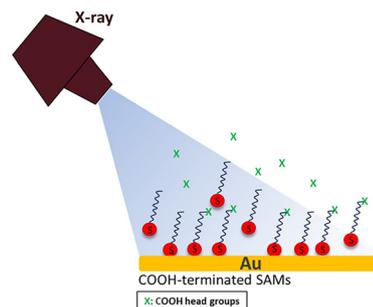
Jianing Wang, Jie Meng, Weiyi Wang\* and Qunxiang Li\*



1901

## X-ray exposure effects on carboxylic-terminated self-assembled monolayers and change in the interface electronic structure

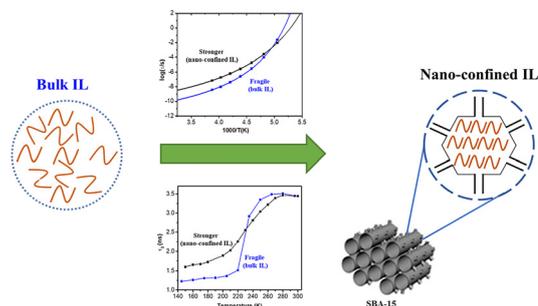
Ahlam R. M. Alharbi, Ingo Köper and Gunther G. Andersson\*



1911

## Reduction in liquid fragility and enhancement in ionic conductivity in the glassy phase of $[\text{Bmlm}][\text{NTf}_2]$ ionic liquid under nano-confinement: PALS and BDS investigations

Shapath Bhandari, Jaideep Mor, Debasis Sen, Jitendra Bahadur, Kanaklata Pandey and Dhanadeep Dutta\*



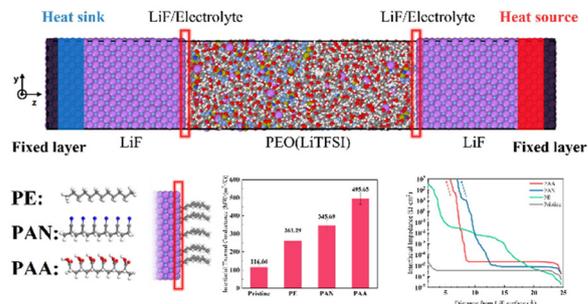


## RESEARCH PAPERS

1976

### Effects of self-assembled monolayers on thermal and lithium-ion transport at the SEI/PEO-based polymer electrolyte interface: a molecular dynamics study

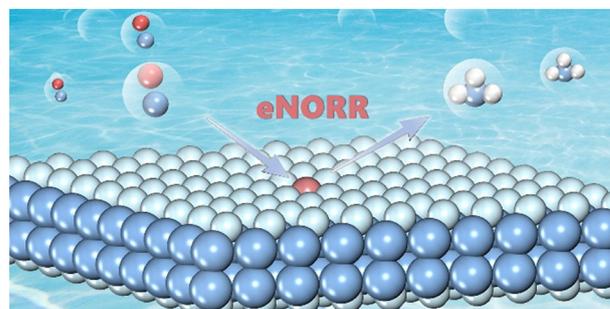
Kang Yi and Dongwei Xu\*



1985

### A silicon single atom anchored on an $\alpha$ -BS monolayer for efficient electrocatalytic nitric oxide reduction to ammonia

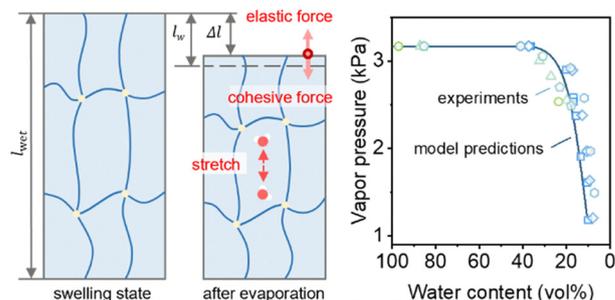
Yongxu Fu, Hu Li, Qingbo Kang, Jiangke Li, Minghui Wu, Lei Liu, Xiaobing Yan, Weichao Wang and Linxia Wang\*



1994

### Modelling of water evaporation in hydrogels considering the state of water in tension

Zehua Yu, Yongshun Ren and Kang Liu\*

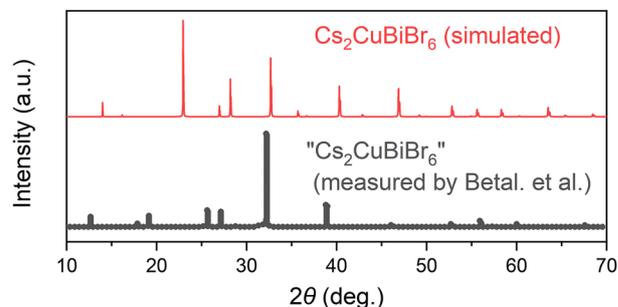


## COMMENTS

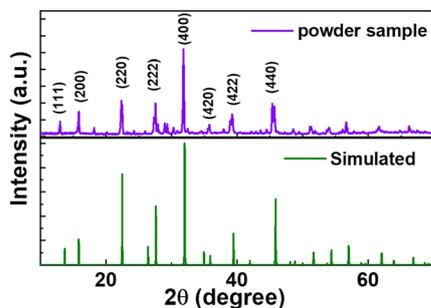
2003

### Comment on "Air-stable double halide perovskite $\text{Cs}_2\text{CuBiBr}_6$ : synthesis and memristor application" by A. Betal, A. Chetia, D. Saikia, K. Karmakar, G. Bera, N. V. Dambhare, A. K. Rath and S. Sahu, *Phys. Chem. Chem. Phys.*, 2025, 27, 3150

Lixia Xiao, Junwei Guo, Gang Tang and Zewen Xiao\*



2006



Reply to the 'Comment on "Air-stable double halide perovskite  $\text{Cs}_2\text{CuBiBr}_6$ : synthesis and memristor application"' by L. Xiao, J. Guo, G. Tang and Z. Xiao, *Phys. Chem. Chem. Phys.*, 2025, 27, DOI: 10.1039/D5CP00194C

Atanu Betal, Anupam Chetia, Dibyajyoti Saikia, Krishnendu Karmakar and Satyajit Sahu\*

