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IN THIS ISSUE

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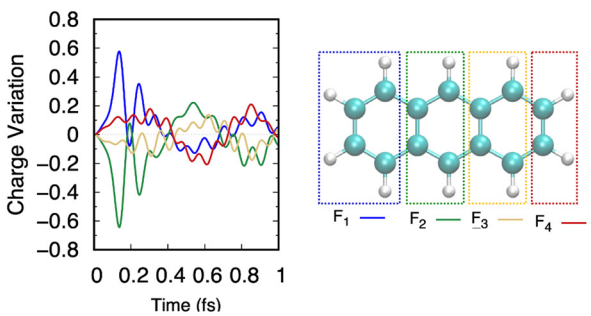
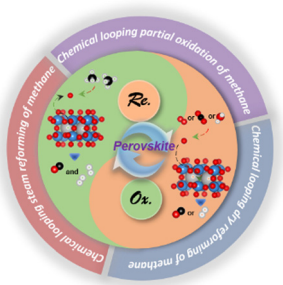
Cover
See Olaf Brummel, Josef Mysliveček *et al.*, pp. 1630–1639. Image reproduced by permission of Josef Mysliveček from *Phys. Chem. Chem. Phys.*, 2024, **26**, 1630.

Inside cover
See Mathias Rapacioli *et al.*, pp. 1499–1515. Image reproduced by permission of Mathias Rapacioli and CNRS-5626 from *Phys. Chem. Chem. Phys.*, 2024, **26**, 1499.

REVIEWS





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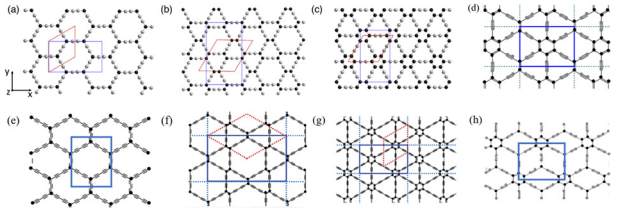

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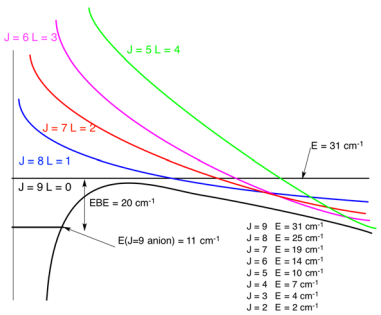
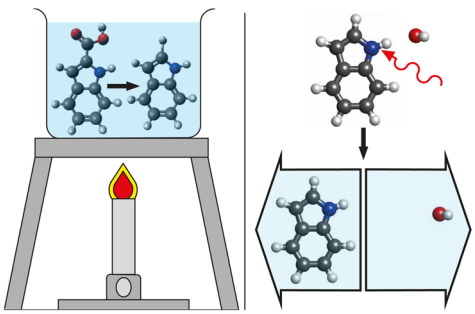
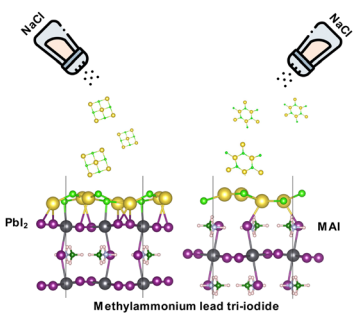


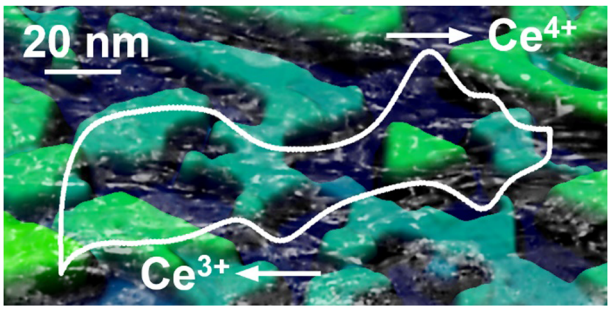


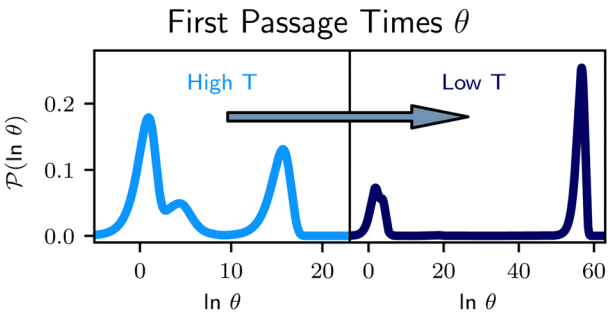
COMMUNICATIONS

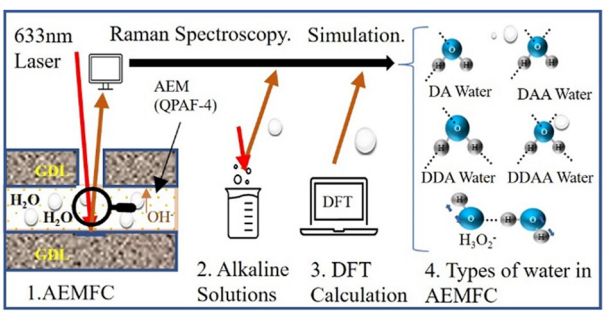


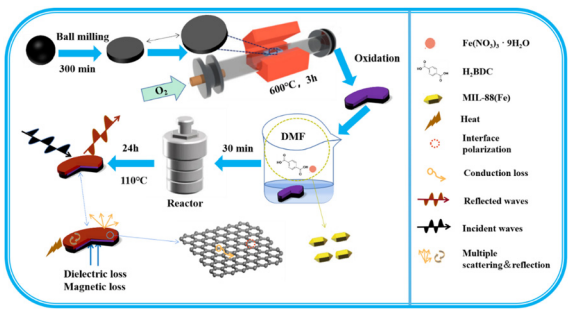
COMMUNICATIONS

RESEARCH PAPERS









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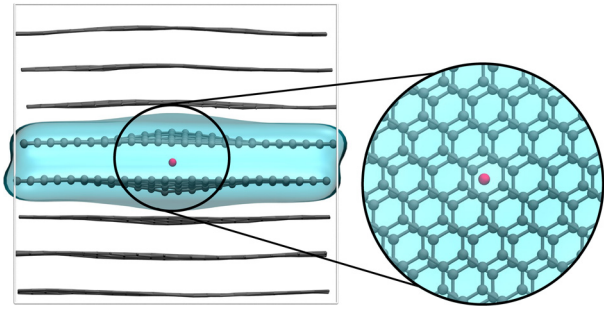

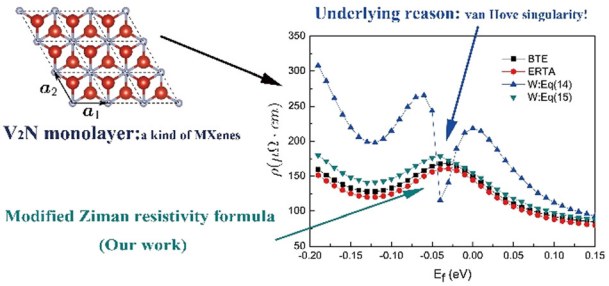

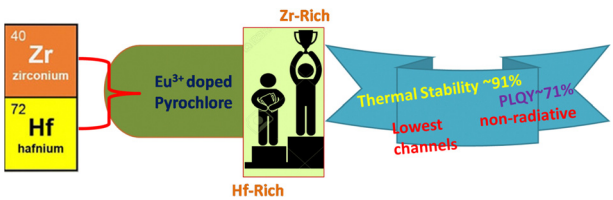

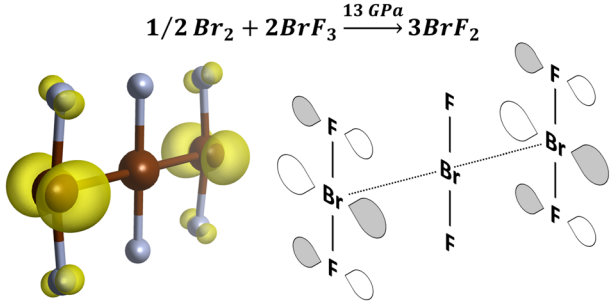

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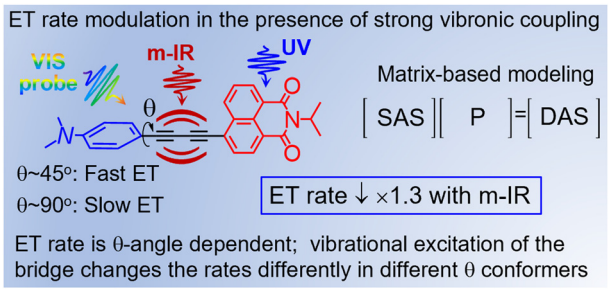

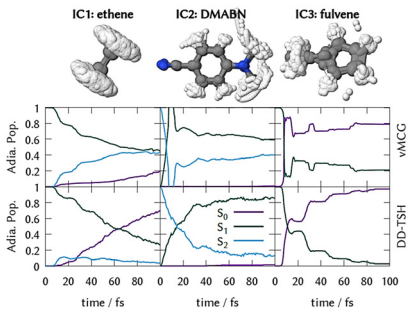

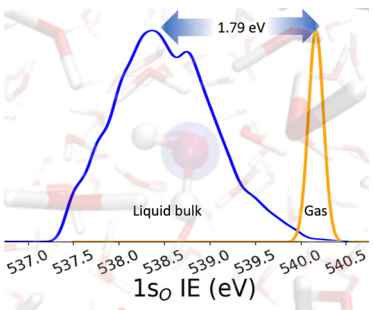

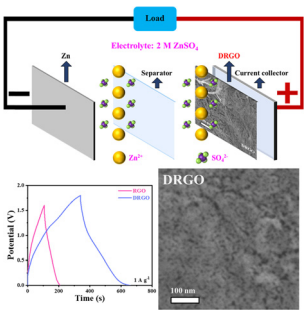

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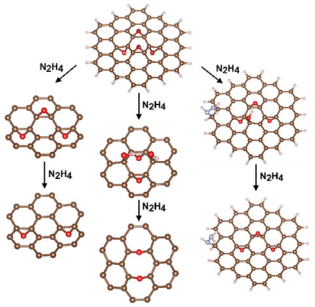
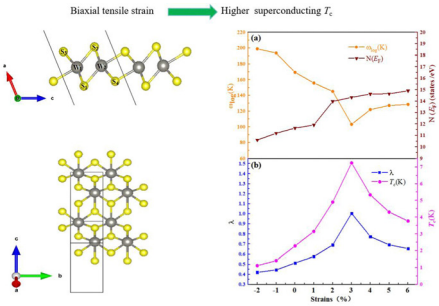
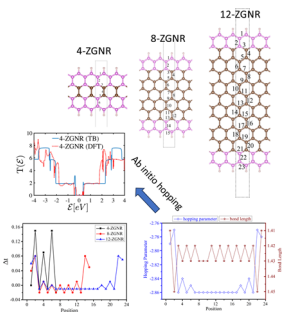
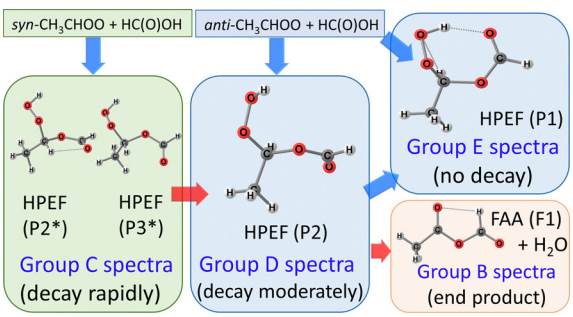
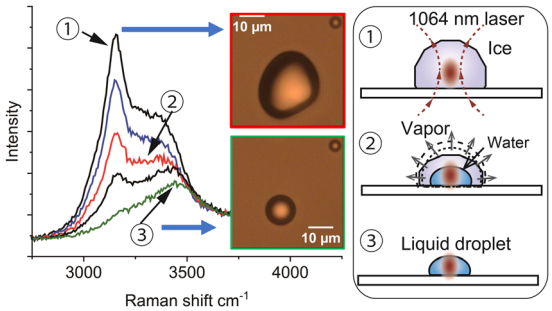








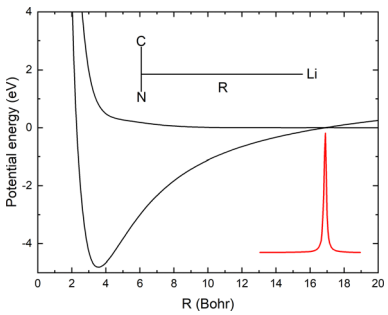
1967



Melting of a single ice microparticle on exposure to focused near-IR laser beam to yield a supercooled water droplet

Shuichi Hashimoto* and Takayuki Uwada

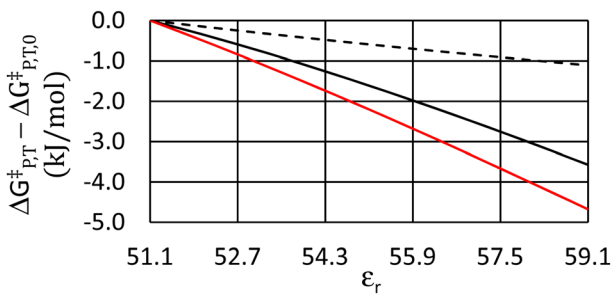
1977



Mutual neutralization in collisions of Li^+ with CN^-

Åsa Larson* and Ann E. Orel

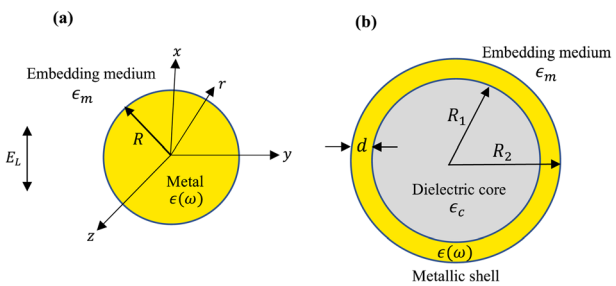
1984



A thermodynamic approach to analyzing relative permittivity and solvent mole fraction models, and application to S_N1 reactions

Floyd L. Wiseman* and Dane W. Scott

1994



Bandwidth of quantized surface plasmons: competition between radiative and nonradiative damping effects

Samar Moustafa, Mohamed K. Zayed, Moustafa Ahmed and Hesham Fares*

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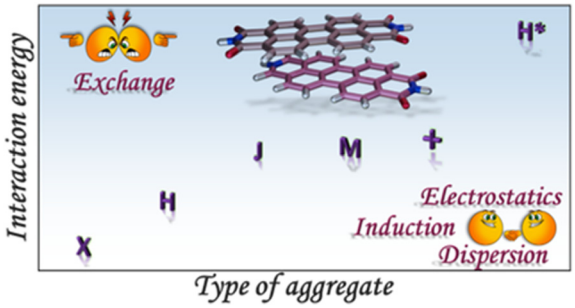
2007

Energy landscape of perylenediimide chromophoric aggregates

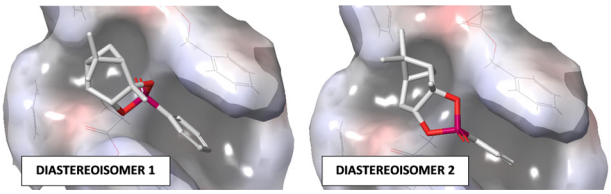
Pallavi Panthakkal Das, Aniruddha Mazumder, Megha Rajeevan, Rotti Srinivasamurthy Swathi* and Mahesh Hariharan*



2016

Exploring the impact of alignment media on RDC analysis of phosphorus-containing compounds: a molecular docking approach

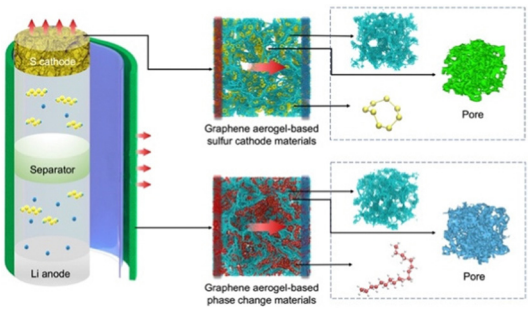
Markéta Christou Tichotová, Lucie Tučková, Hugo Kocek, Aleš Růžička, Michal Straka and Eliška Procházková*



2025

Thermal transport properties of graphene aerogel as an advanced carrier for enhanced energy storage

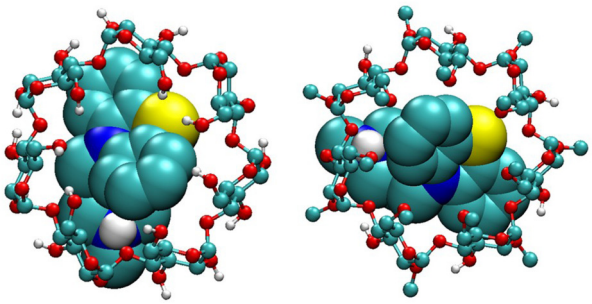
Jieren Song,* Xianghua Xu and Xingang Liang



2035

Host–guest systems for the SAMPL9 blinded prediction challenge: phenothiazine as a privileged scaffold for binding to cyclodextrins

Brenda Andrade, Ashley Chen and Michael K. Gilson*



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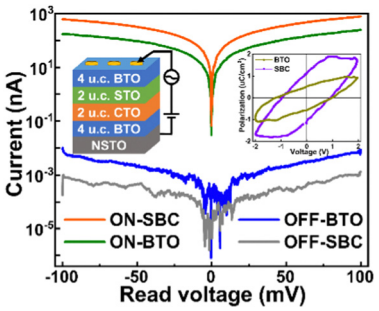

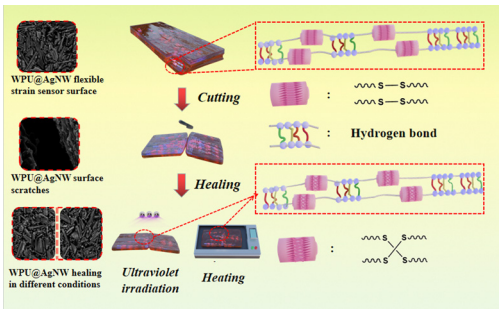

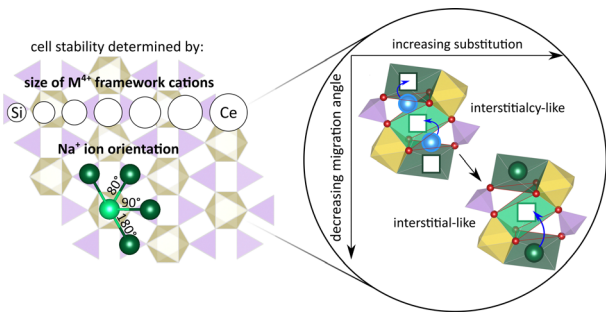

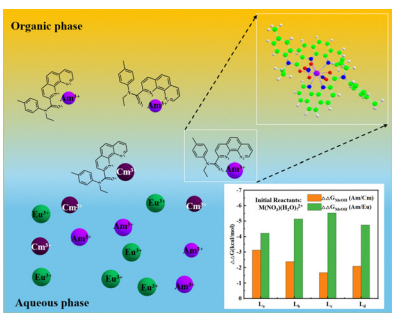

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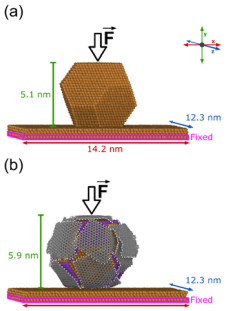

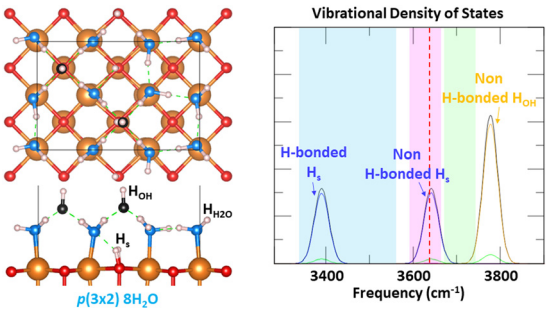

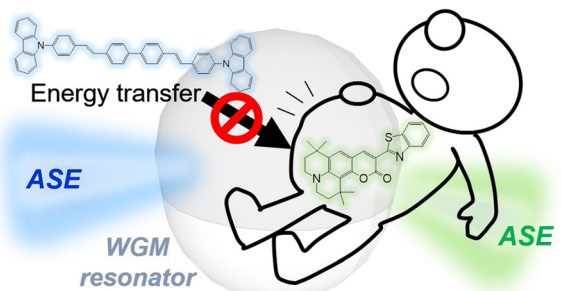

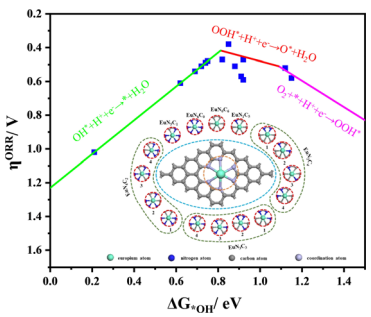

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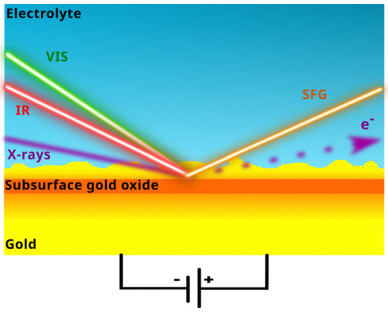

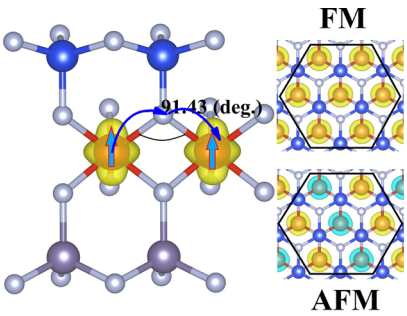

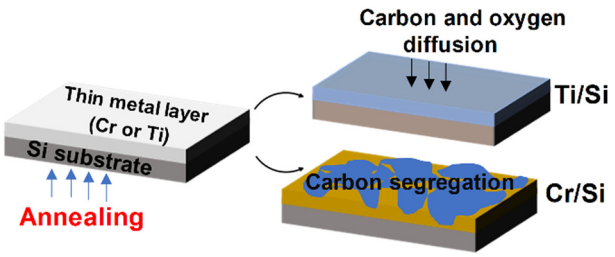

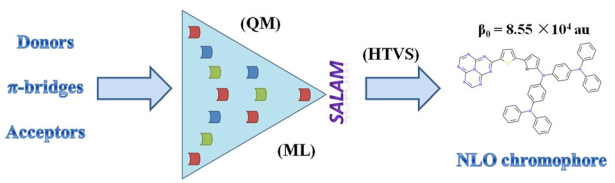

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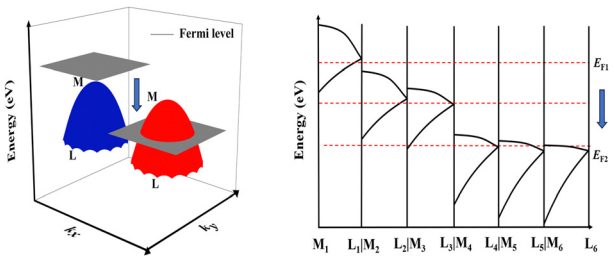
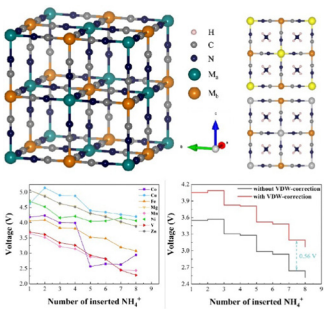


Theoretical study of CDW phases for bulk NbX_2 (X = S and Se)

Hongwei Du, Zhenyi Jiang,* Jiming Zheng,* Xiaodong Zhang, Wenxuan Wang and Zhiyong Zhang

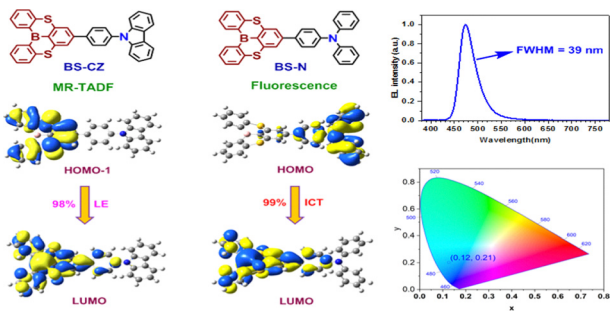
2387



Element screening of metal sites in Fe-based Prussian blue framework materials for ammonium ion battery applications: a first-principles study

Yu Zhang, Junjie Xing, Bo Zhang, Likai Tong and Xiuli Fu*

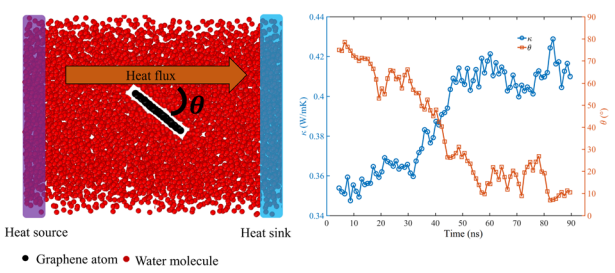
2395



B-embedded disulfide-bridged π-conjugated compounds: structures and optical tuning

Kaishun Ye, Gang Li, Feiyang Li, Chao Shi,* Zhen Jiang, Fuzheng Zhang, Qiuxia Li,* Jie Su, Dandan Song* and Aihua Yuan

2402



Coupling at the molecular scale between the graphene nanosheet and water and its effect on the thermal conductivity of the nanofluid

Xiong Pan, Hanhui Jin,* Xiaoke Ku, Yu Guo and Jianren Fan

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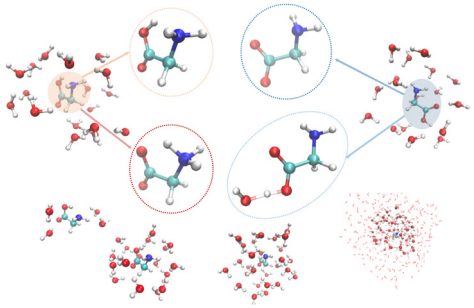

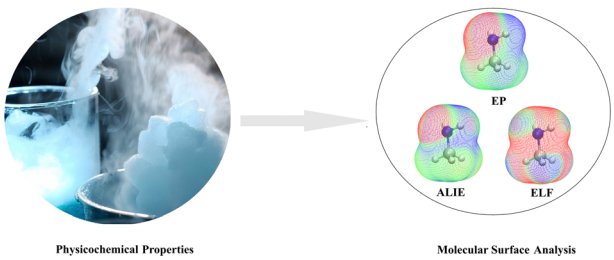

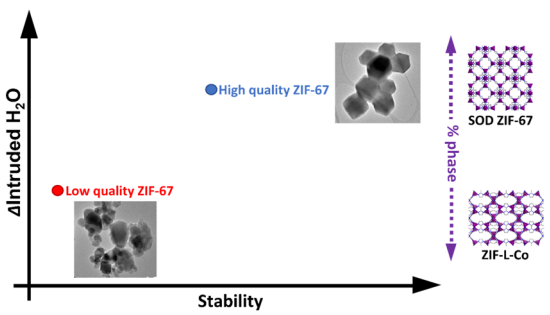

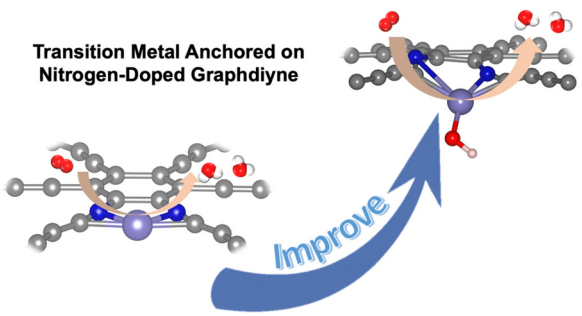

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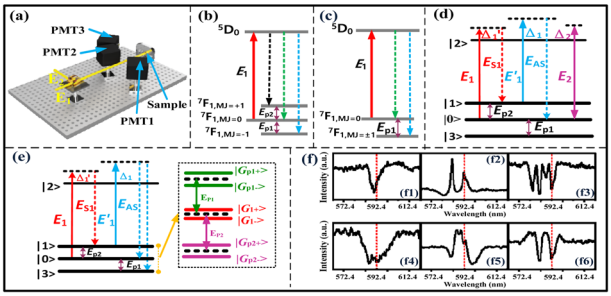

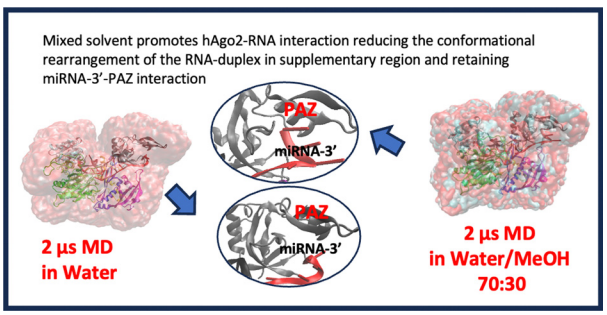

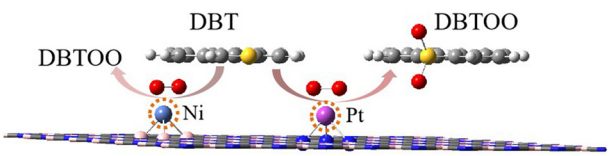

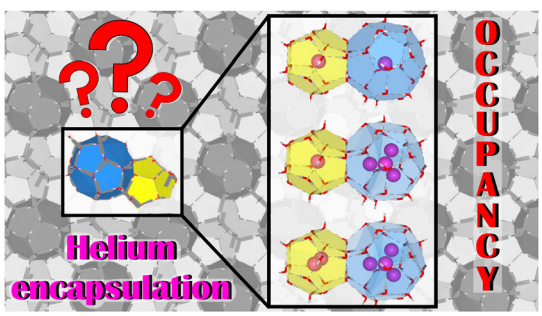

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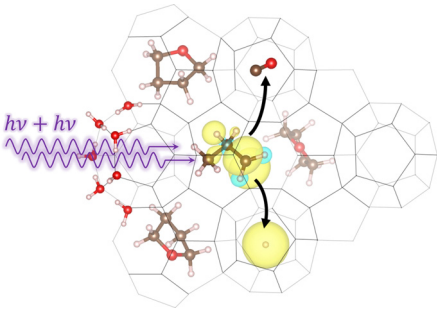

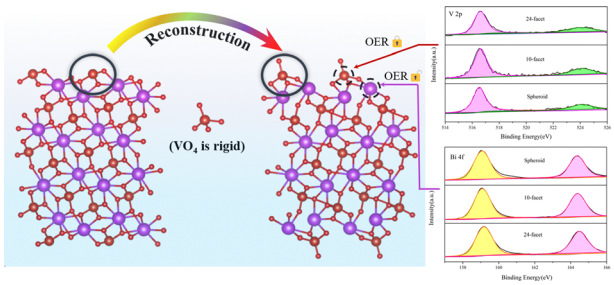

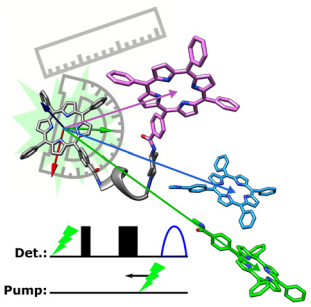

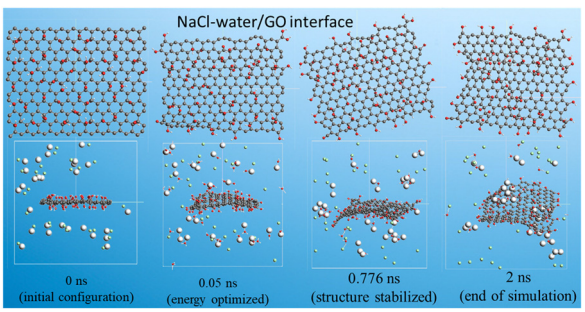

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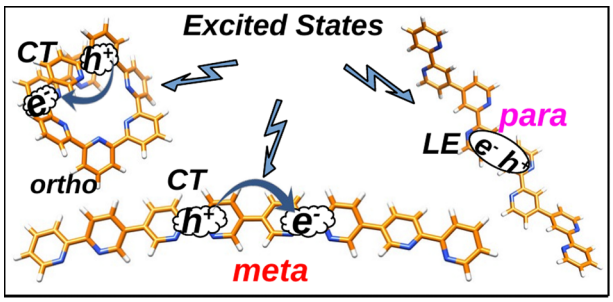

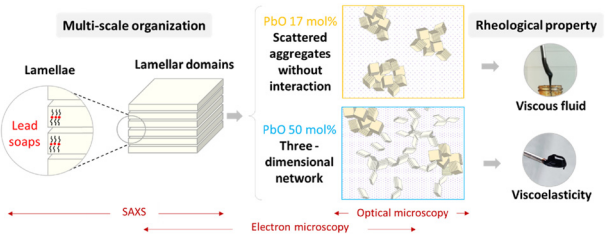

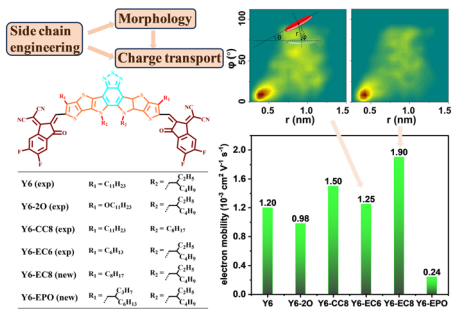

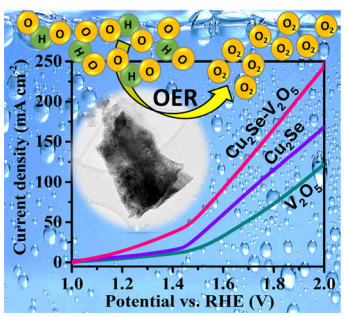

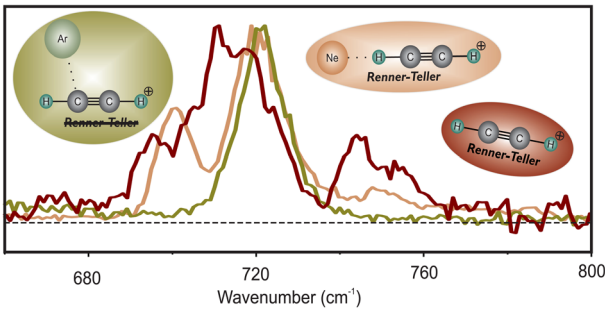

Leak-out spectroscopy as alternative method to rare-gas tagging for the Renner–Teller perturbed $HCCH^+$ and $DCCD^+$ ions

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