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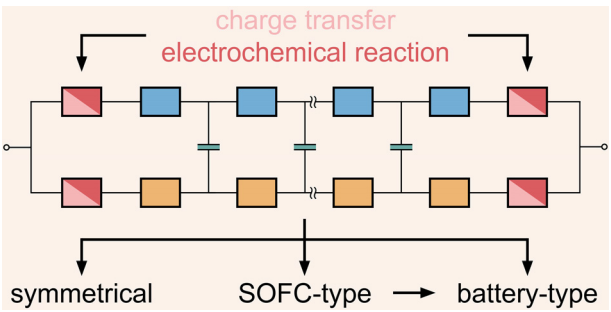
TUTORIAL REVIEW



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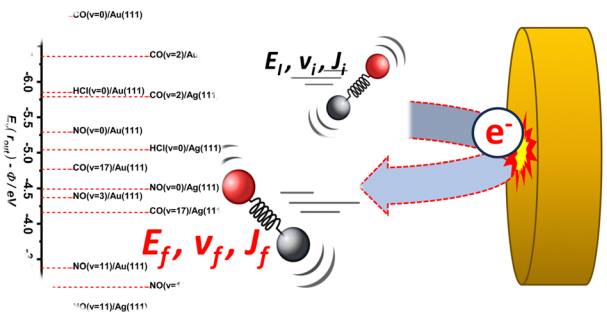

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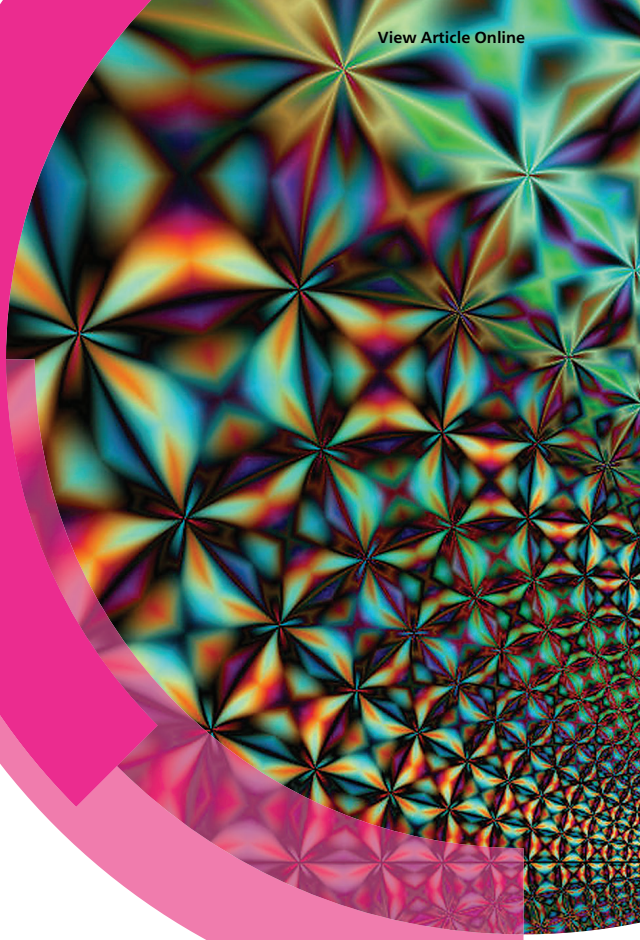

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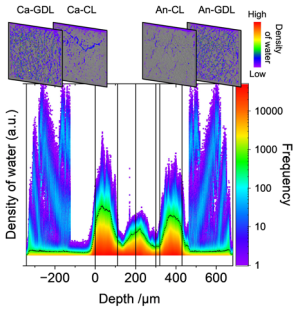

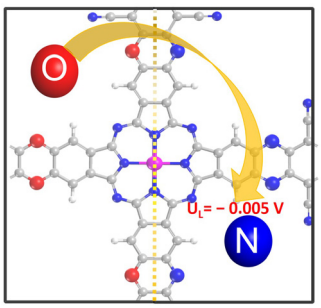

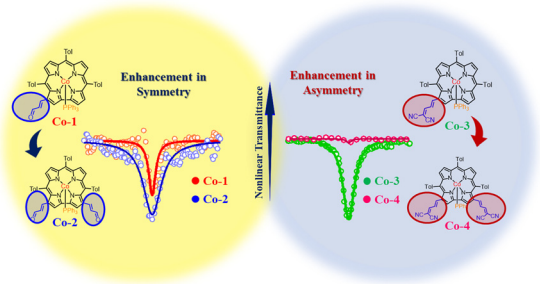

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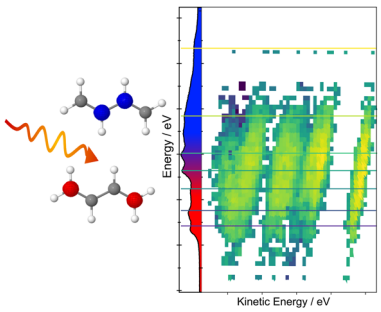

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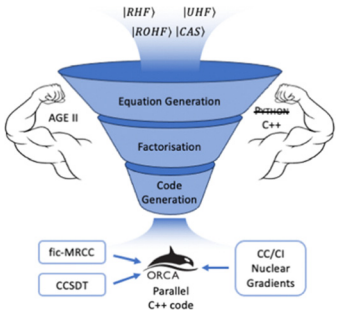

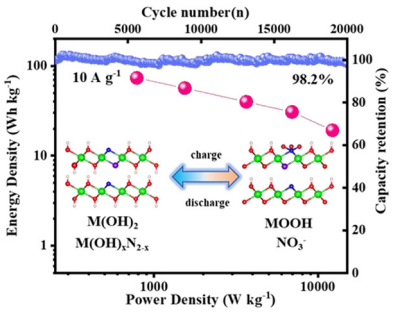

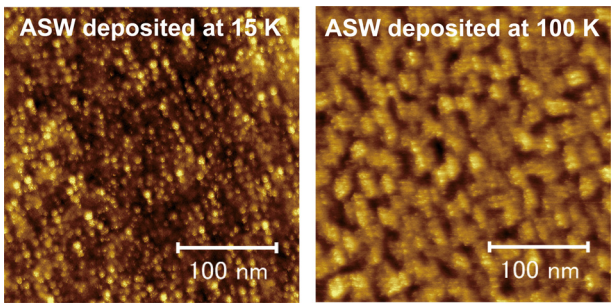

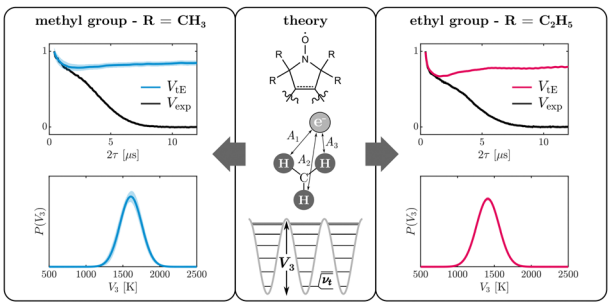

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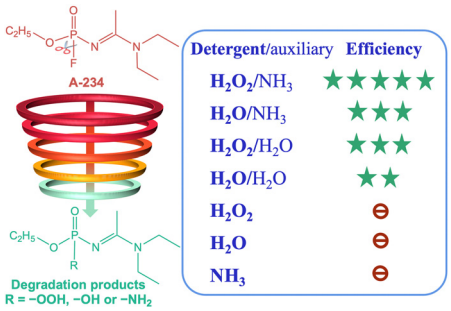

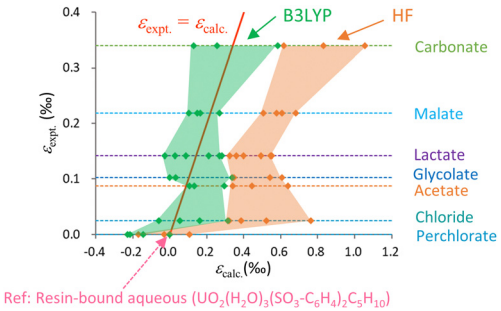

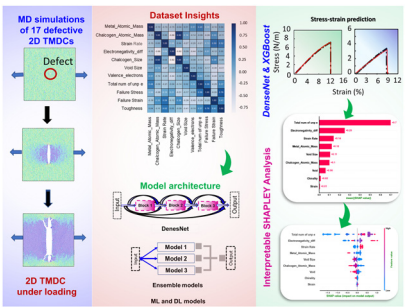

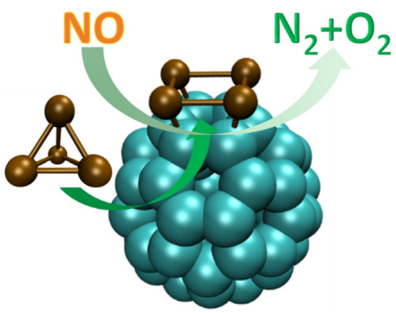

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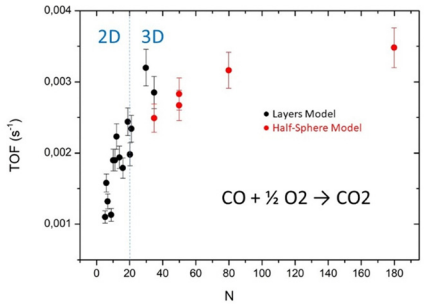
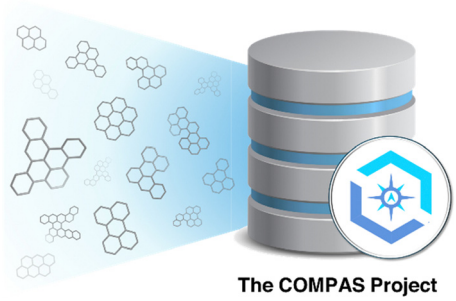


A molecular beam study of CO oxidation on Pd clusters supported on alumina: the effect of cluster size

Georges Sitja* and Claude R. Henry*

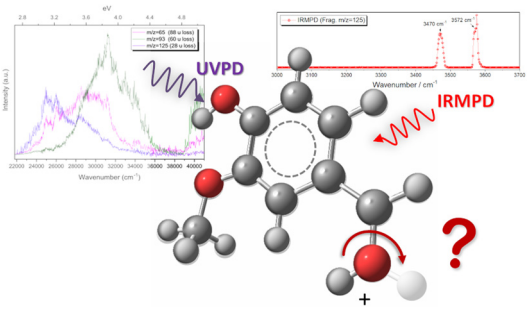
15344



COMPAS-3: a dataset of *peri*-condensed polybenzenoid hydrocarbons

Alexandra Wahab and Renana Gershoni-Poranne*

15358



Vibrational and electronic spectra of protonated vanillin: exploring protonation sites and isomerisation

Alejandro Gutiérrez-Quintanilla, Baptiste Moge, Isabelle Compagnon and Jennifer A. Noble*

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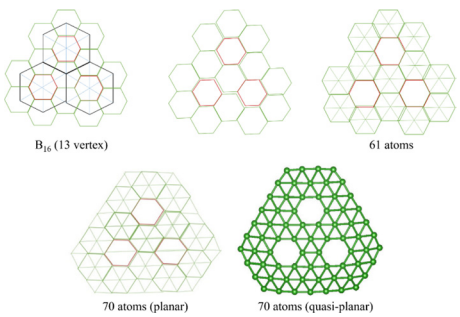

A topological path to the formation of a quasi-planar B_{70} boron cluster and its dianion

Pinaki Saha, Fernando Buendía, Long Van Duong and Minh Tho Nguyen*

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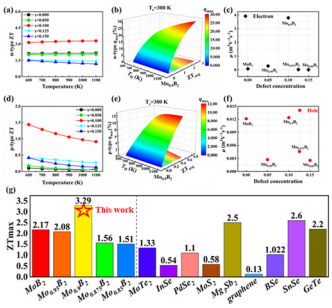
Two-dimensional $Mo_{1-x}B_2$ with ordered metal vacancies obtained for advanced thermoelectric applications based on first-principles calculations

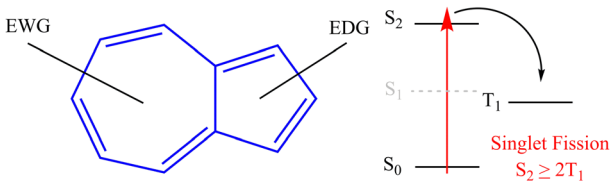
Jie Pu, Ziyu Hu* and Xiaohong Shao*



15386

Designing potentially singlet fission materials with an anti-Kasha behaviour

Ricardo Pino-Rios,* Rodrigo Báez-Grez, Dariusz W. Szczepanik and Miquel Solá*



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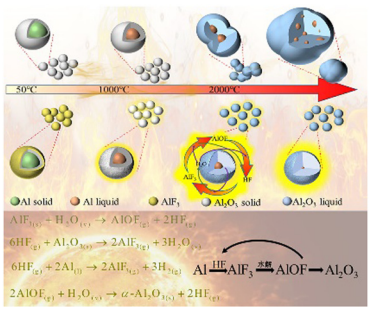
Enhancing the combustion of nAl with AlF_3 coating: gas–solid reaction mechanism for reducing combustion agglomeration of Al powder

Chen Shen, Shi Yan,* Jie Yao, Hui Ren, Xueyong Guo, Jianxin Nie, Yapeng Ou, Qingjie Jiao and Yunjun Luo



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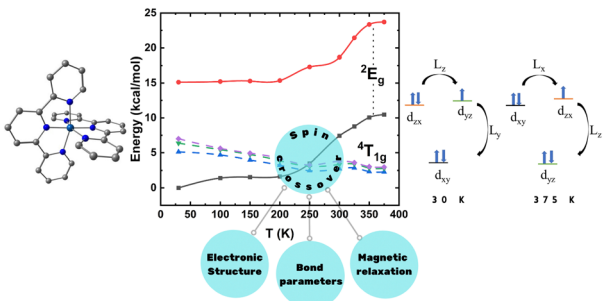
Ab initio calculation of magnetic anisotropy and thermal spin transition in the variable temperature crystal conformations of $[Co(terpy)_2]^{2+}$

Moromi Nath, Shalini Joshi and Sabyashachi Mishra*



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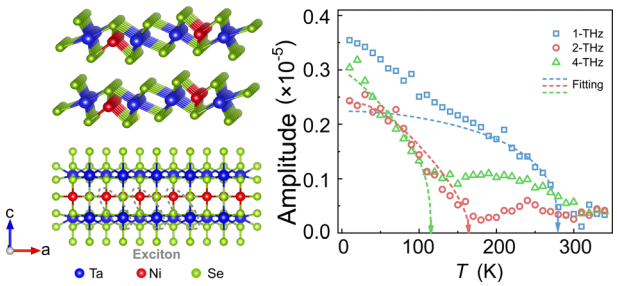

Multiple coherent amplitude modes and exciton–phonon coupling in quasi-one-dimensional excitonic insulator Ta_2NiSe_5

Yaohua Jiang, Yang Mi,* Jia Guo,* Zixuan Wang, Ning Zhang, Bo Liu and Sheng-Nian Luo

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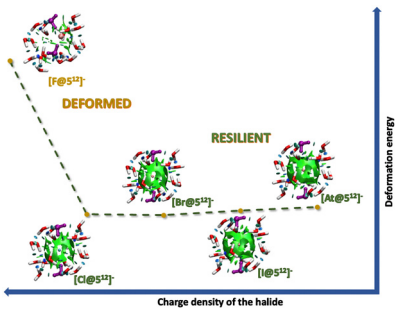

Encapsulation of charged halogens by the 5^{12} water cage

Sara Gómez,* Elizabeth Flórez, Nancy Acelas, Chiara Cappelli, Cacier Hadad and Albeiro Restrepo*

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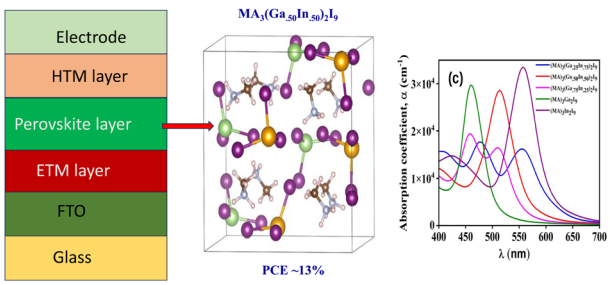

Ga and In-based hybrid halide perovskites as an alternative to Pb: a first principles study

Tridip Chutia, Tanmoy Kalita, Uddipana Saikia and Dhruba Jyoti Kalita*

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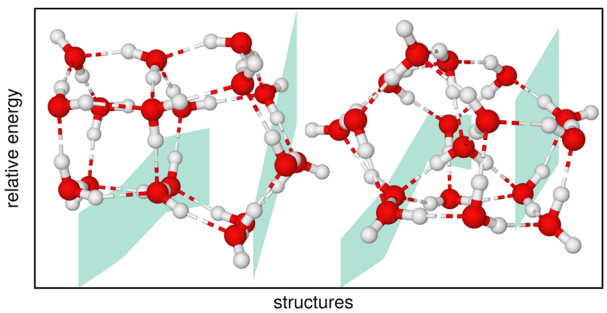

On the brink of self-hydration: the water heptadecamer

Bernd Hartke

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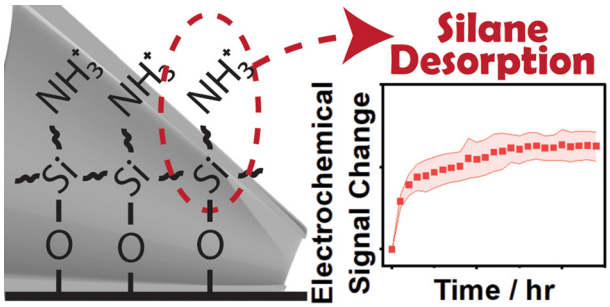

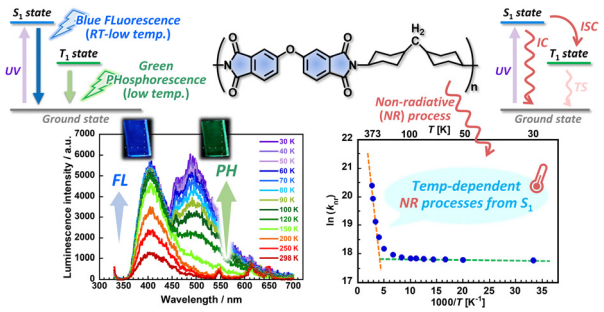

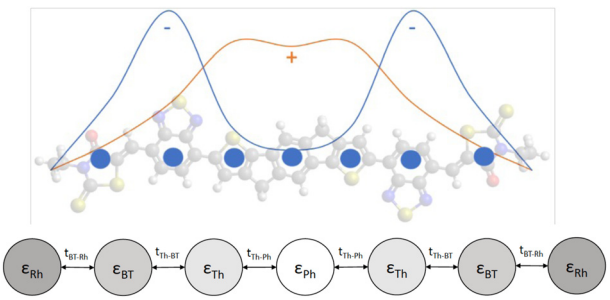

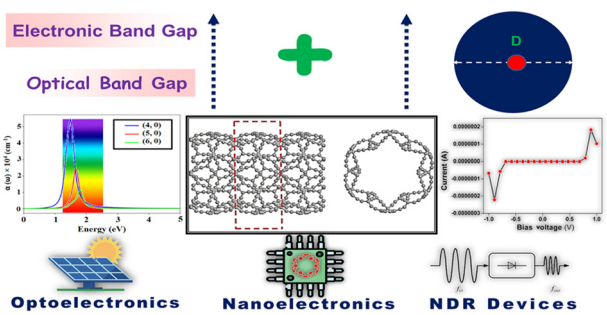

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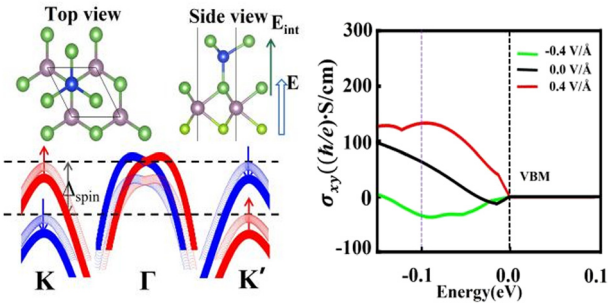

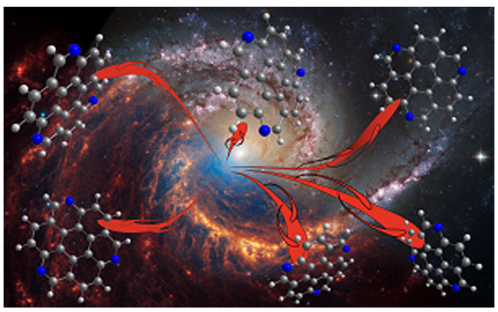

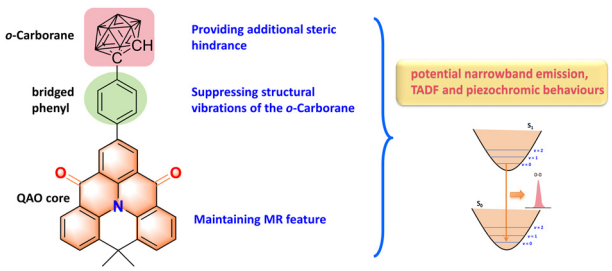

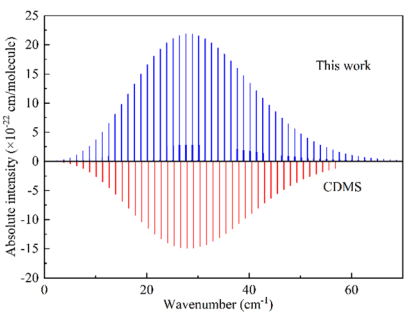

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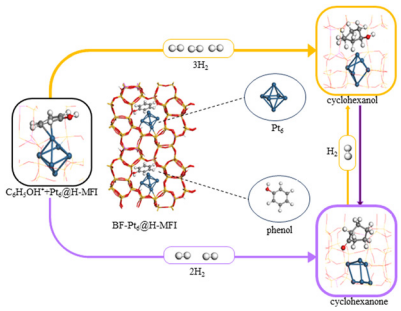

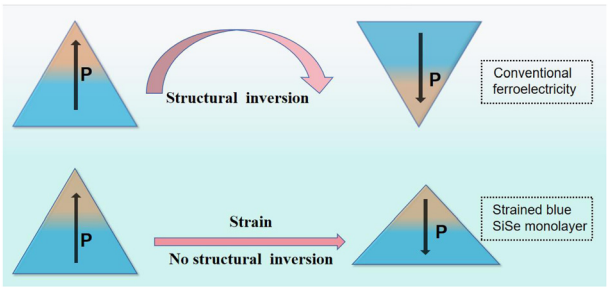

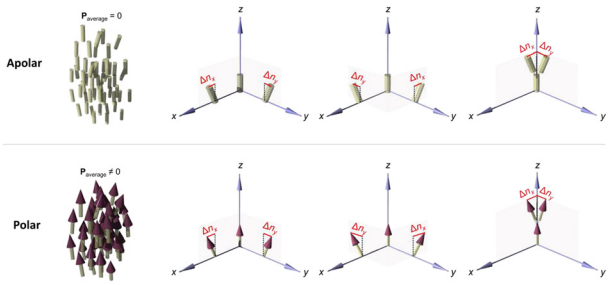

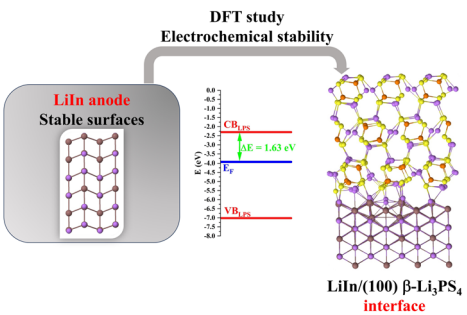

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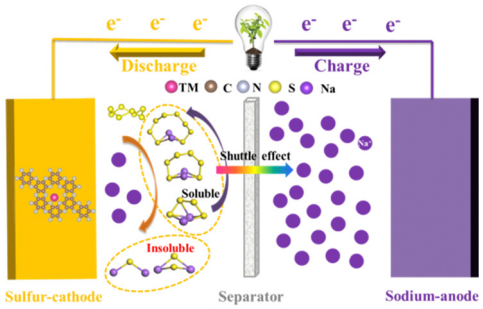
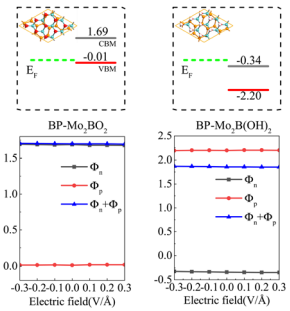


Single-atom catalysts based on C_2N for sulfur cathodes in Na–S batteries: a first-principles study

Wanlin Xu, Tengrui Feng, Jiezhen Xia, Rong Cao and Qi Wu*

15666



Surface-engineered Mo_2B: a promising electrode material for constructing Ohmic contacts with blue phosphorene for electronic device applications

Jingying Yang, Xiang Liu, Xiaohui Deng, Zhenkun Tang and Liemao Cao*

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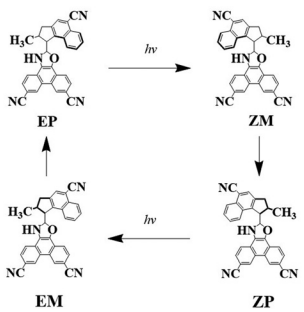

Advanced theoretical design of light-driven molecular rotary motors: enhancing thermal helix inversion and visible-light activation

Weiliang Shi, Jianzheng Ma, Chenwei Jiang* and Tetsuya Taketsugu*

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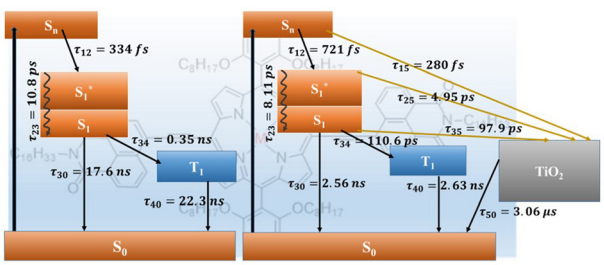

Hot carrier dynamics in metalated porphyrin–naphthalimide thin films

Md Soif Ahmed, Sudhanshu Kumar Nayak, Botta Bhavani, Dipanjan Banerjee, Seelam Prasanthkumar, Lingamallu Giribabu, Venugopal Rao Soma and Sai Santosh Kumar Raavi*

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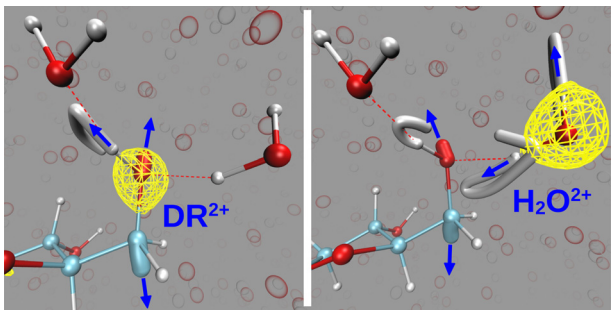

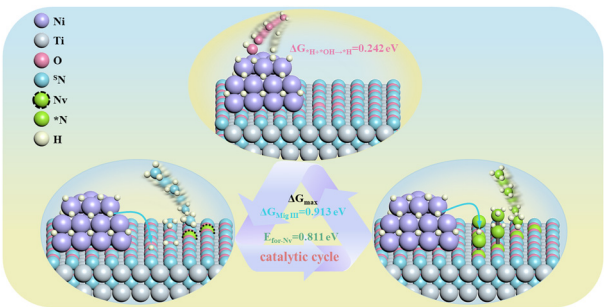

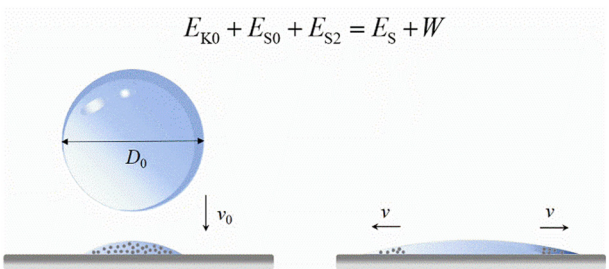

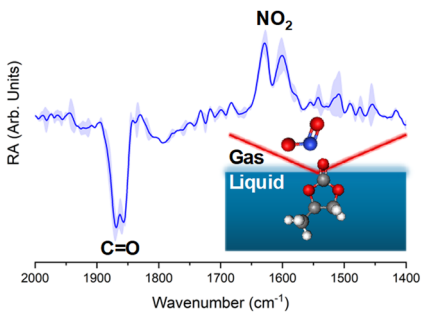

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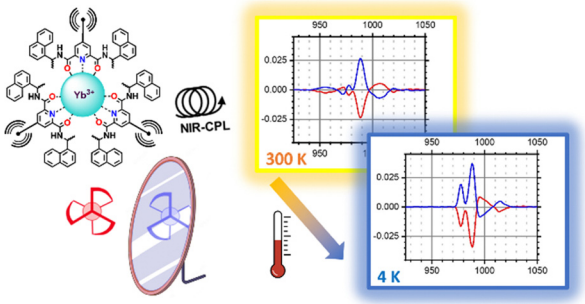

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