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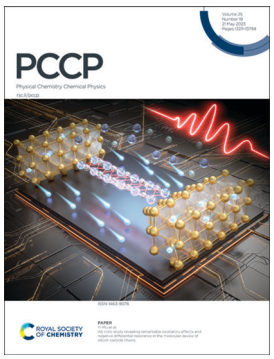

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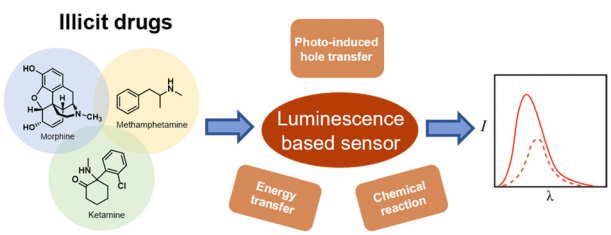
See Sunil Saxena *et al.*, pp. 13275–13288. Image reproduced by permission of Sunil Saxena from *Phys. Chem. Chem. Phys.*, 2023, **25**, 13275.

TUTORIAL REVIEW

PERSPECTIVE



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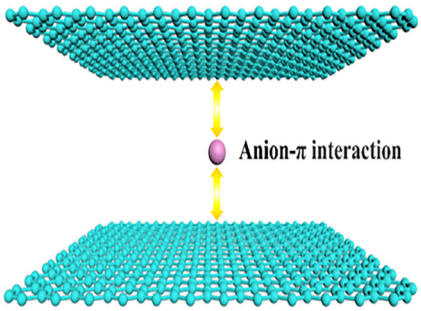

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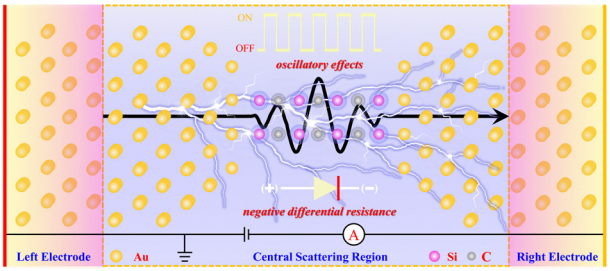

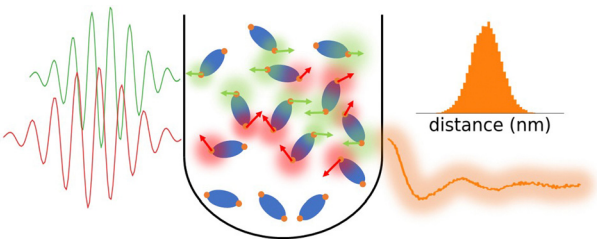

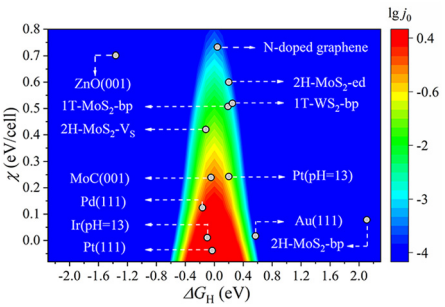

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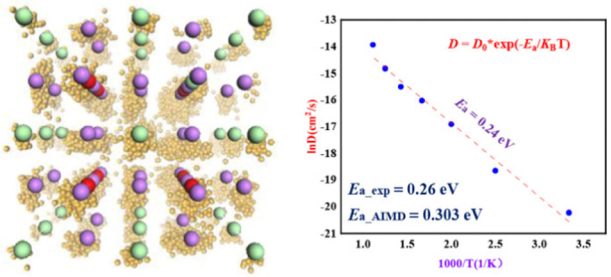

Li ion diffusion behavior of Li_3OCl solid-state electrolytes with different defect structures: insights from the deep potential model

Zhou Zhang, Zhongyun Ma* and Yong Pei*

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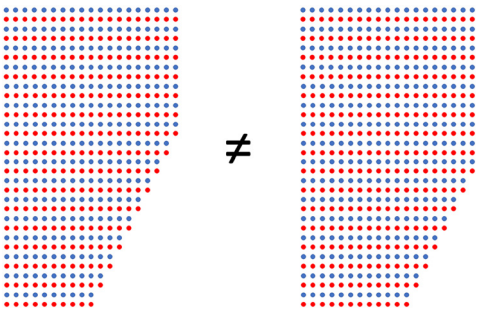

The shape effect and its consequences for polar surfaces and for heterogeneous catalysis

Michael Springborg,* Meijuan Zhou and Bernard Kirtman

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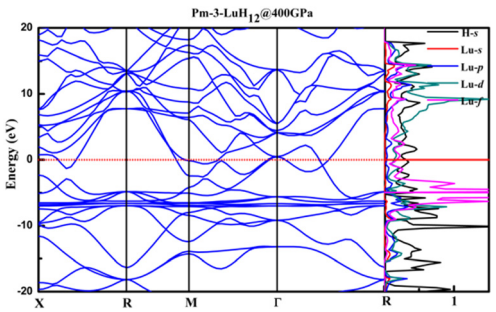

Pressure-induced stability and superconductivity in LuH_{12} polyhydrides

Junyi Du, Weiguo Sun, Xiaofeng Li and Feng Peng*

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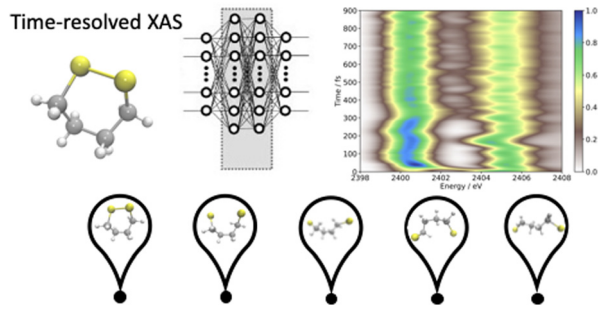

An on-the-fly deep neural network for simulating time-resolved spectroscopy: predicting the ultrafast ring opening dynamics of 1,2-dithiane

Clelia Middleton, Conor D. Rankine and Thomas J. Penfold*

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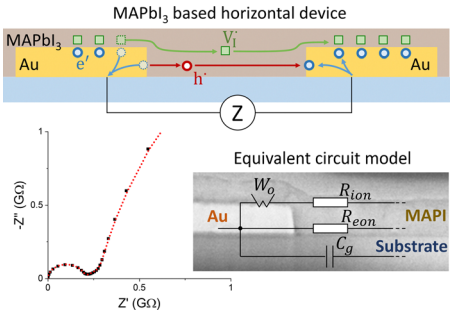
Ionic and electronic polarization effects in horizontal hybrid perovskite device structures close to equilibrium

Davide Moia,* Mina Jung, Ya-Ru Wang and Joachim Maier



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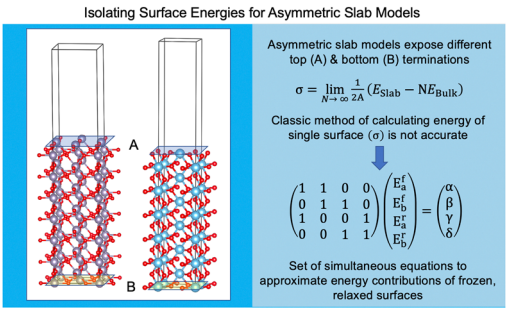
A method of calculating surface energies for asymmetric slab models

Natalie M. Stuart* and Karl Sohlberg



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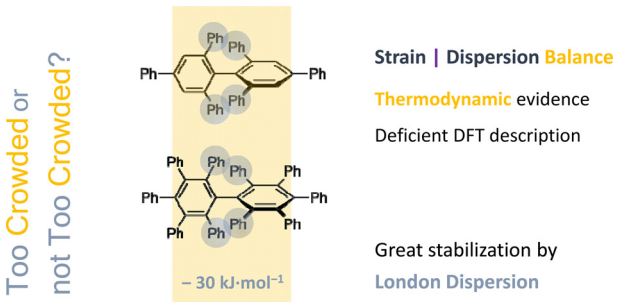
How great is the stabilization of crowded polyphenylbiphenyls by London dispersion?

Carlos F. R. A. C. Lima, Joel T. Mague, Yuchen Du, Robert A. Pascal Jr and Luís M. N. B. F. Santos*



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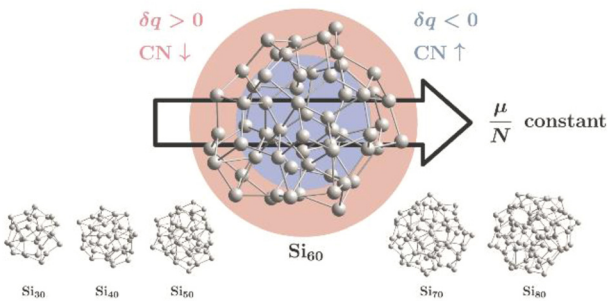
Scaling of the permanent electric dipole moment in isolated silicon clusters with near-spherical shape

Filip Rivic,* Andreas Lehr and Rolf Schäfer



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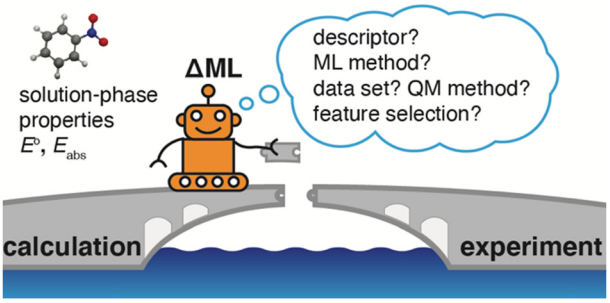
Δ-Machine learning for quantum chemistry prediction of solution-phase molecular properties at the ground and excited states

Xu Chen, Pinyuan Li, Eugen Hruska and Fang Liu*



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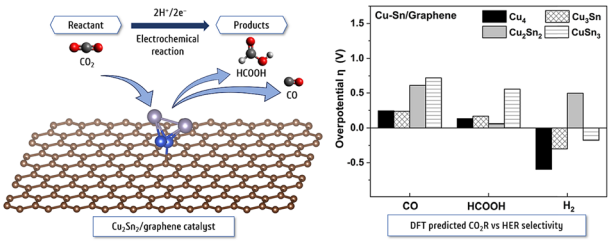
Adsorption, activation, and conversion of carbon dioxide on small copper–tin nanoclusters

Akshayini Muthuperiyanayagam, Azeem Ghulam Nabi, Qi Zhao, Aman-ur-Rehman and Devis Di Tommaso*



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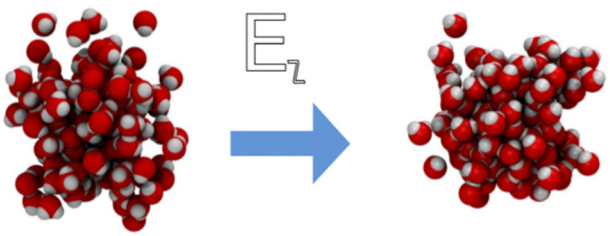
Vibrational dynamics of liquid water in an external electric field

Deepak Ojha* and Thomas D. Kühne



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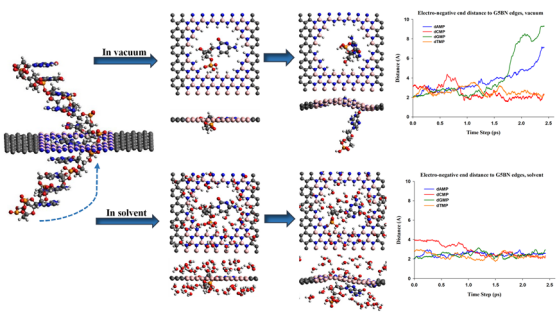
Exploring the dynamics of DNA nucleotides in graphene/h-BN nanopores: insights from *ab initio* molecular dynamics

Ali Kiakojouri, Irmgard Frank and Ebrahim Nadimi*



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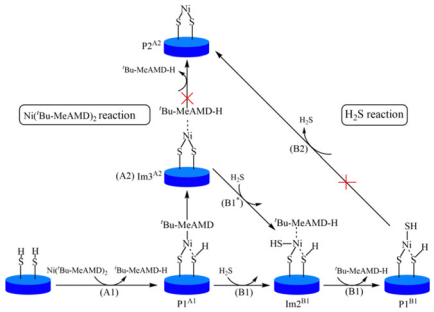
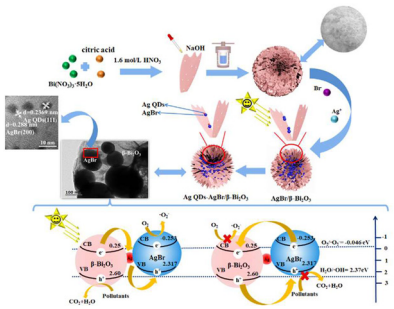


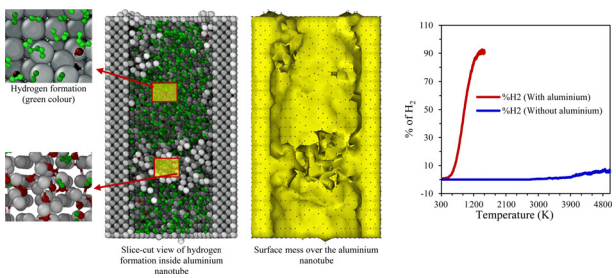
Reaction mechanism of nickel sulfide atomic layer deposition using bis(*N*,*N*′-di-*tert*-butylacetamidinato)nickel(II) and hydrogen sulfide

Xu Zhang, Zhongchao Zhou, Rui Xu, Jiayi Guo, Lina Xu,* Yihong Ding, Hongping Xiao, Xinhua Li, Aidong Li and Guoyong Fang*



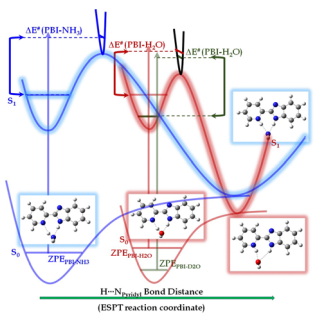
Construction of a Z-scheme heterojunction bifunctional photocatalyst with Ag-modified AgBr embedded in β-Bi_2O_3 flowers

Xin Guan, Xiao-li Wang, Xue-wen Zhu, Hui Yu,* Ming Yang, Xiang-ting Dong,* Ying Yang* and Long Xia*



Aluminum nanotubes as an efficient catalyst for hydrogen production *via* thermochemical water splitting: a reactive molecular dynamics simulation

Sunil Kumar* and Ranjan K. Sahu



Excited-state deactivation *via* solvent-to-chromophore proton transfer in an isolated 1 : 1 molecular complex: experimental validation by measuring the energy barrier and kinetic isotope effect

Saurabh Khodia, Ramesh Jarupula, Simran Baweja, Muhammed Shabeeb, Bhavika Kalal and Surajit Maity*

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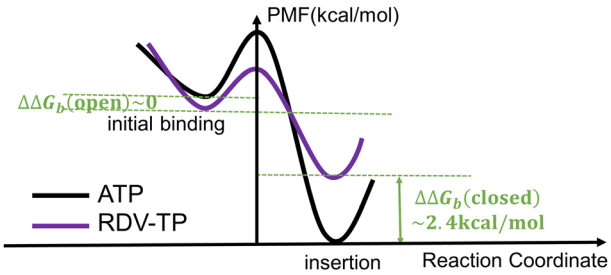

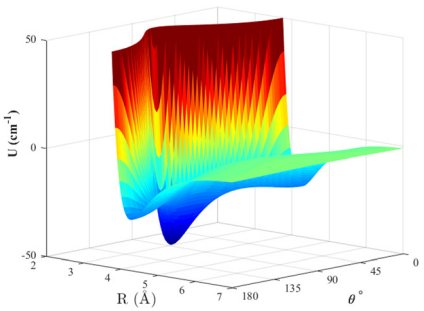

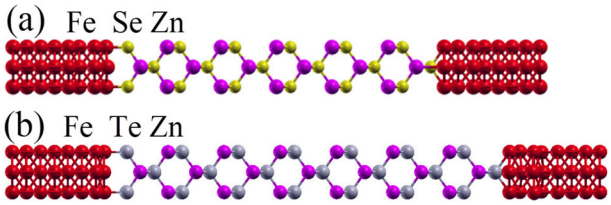

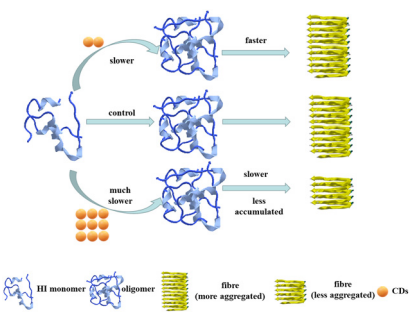

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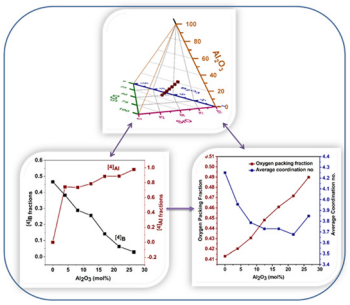

An investigation of Al_2O_3 induced variations in the structural parameters in strontium borosilicate glasses using solid state NMR

Kavya Illath, Prasanta K. Ojha, Sangram K. Rath and T. G. Ajithkumar*

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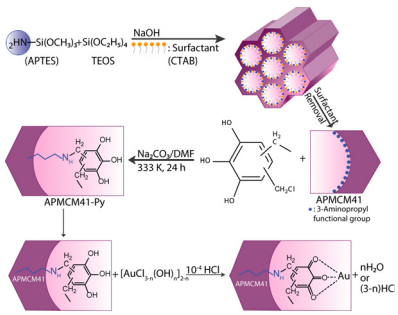

Optimization of Au(III) adsorption by the Taguchi method using pyrogallol functionalized silica nanoparticles

Mustafa Can,* Engin Deniz Parlar, Mustafa Akçil, Abdülkadir Kızılarslan, Semra Boran, Abdullah Hulusi Kökçam and Özer Uygun

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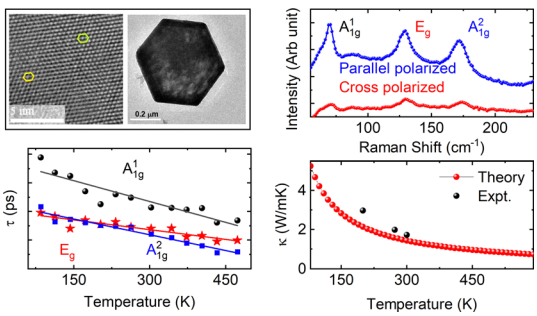

Lattice thermal conductivity of topological insulator Bi_2Se_3 nanocrystals: comparison from theoretical and experimental

Vipin K. E., Soumendra Kumar Das and Prahallad Padhan*

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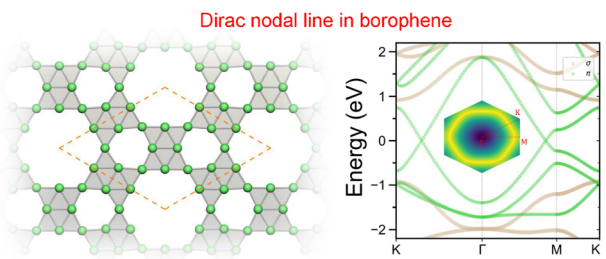

A two-dimensional borophene monolayer with ideal Dirac nodal-line fermions

Chengyong Zhong,* Xuelian Li, Chunbao Feng and Peng Yu*

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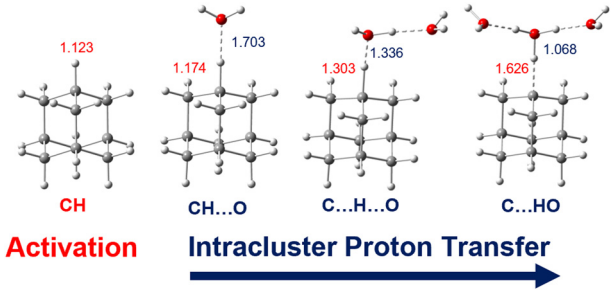

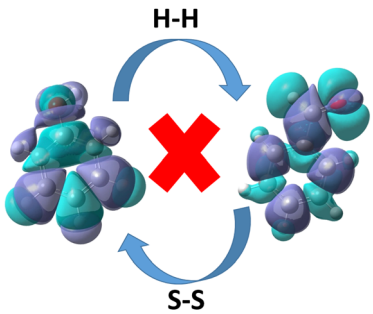

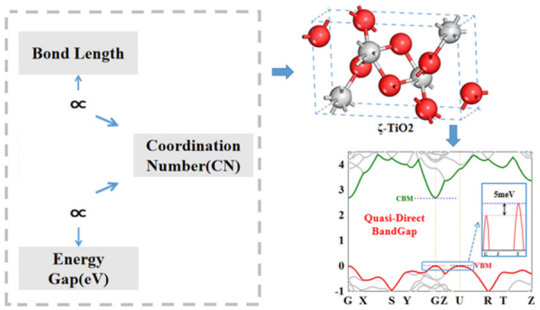

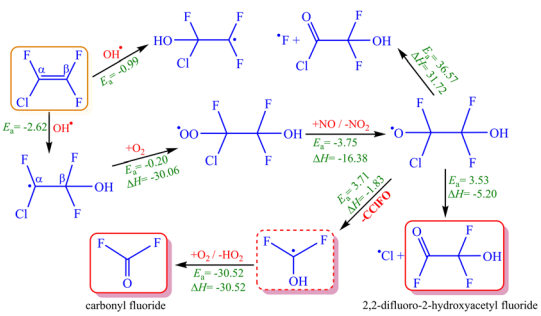

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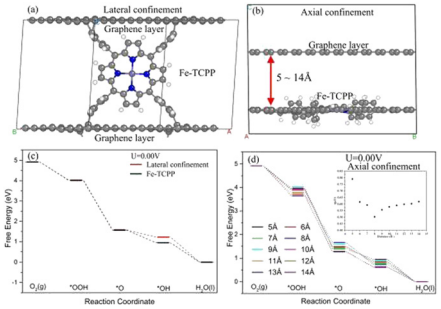

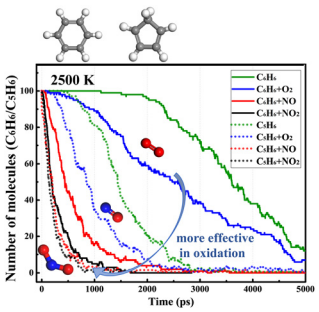

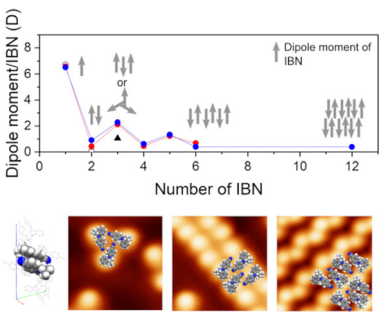

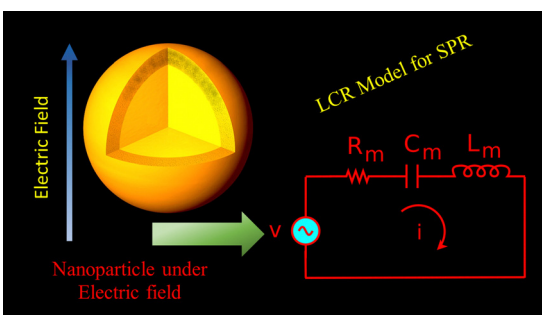

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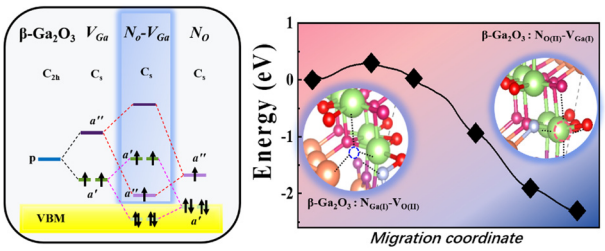

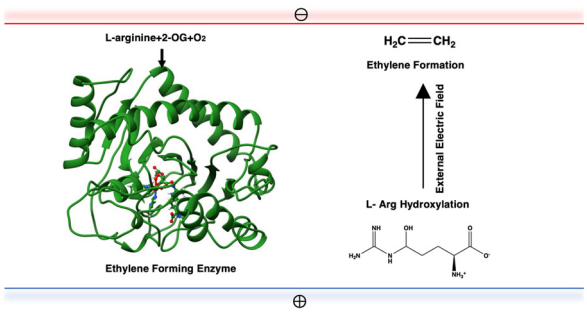

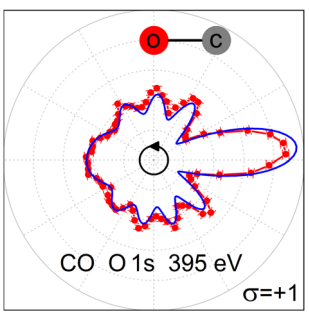

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