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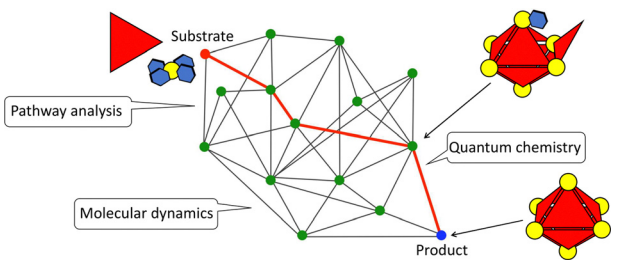
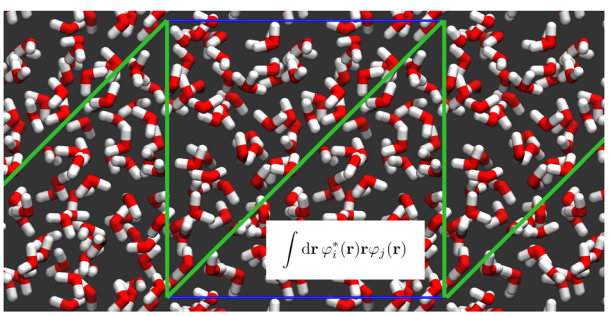
PERSPECTIVES





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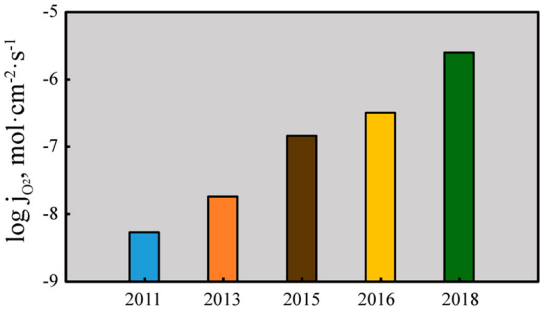

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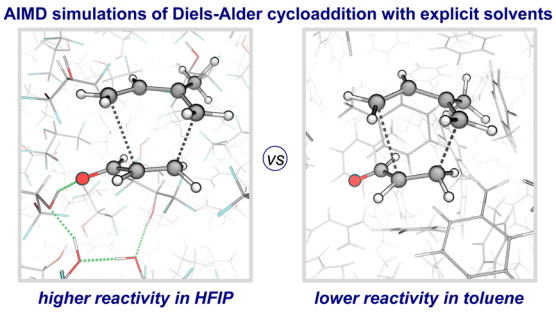

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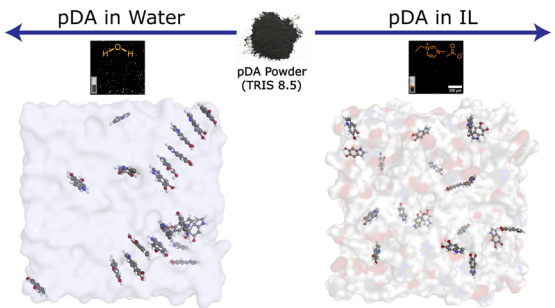

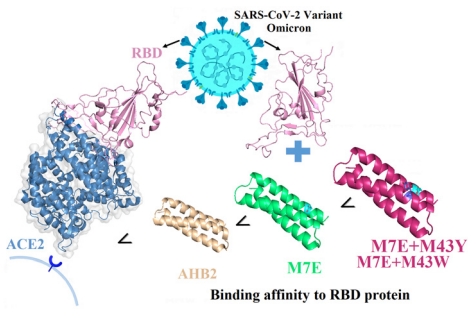

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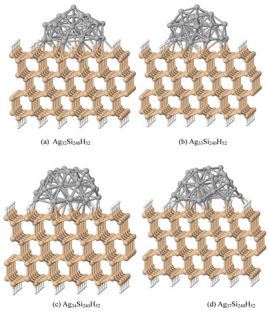

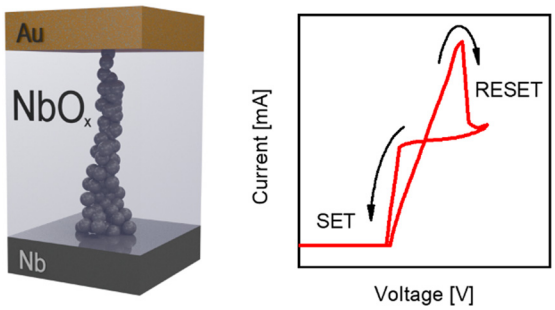

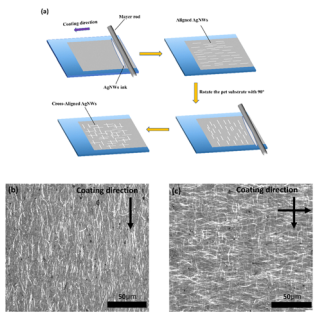

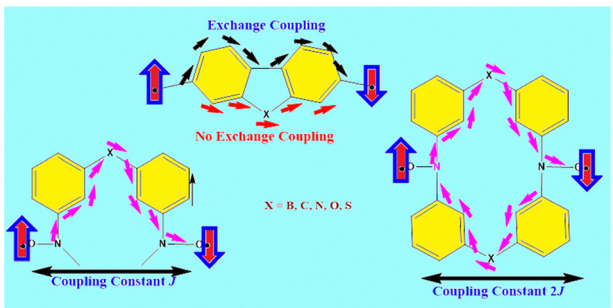

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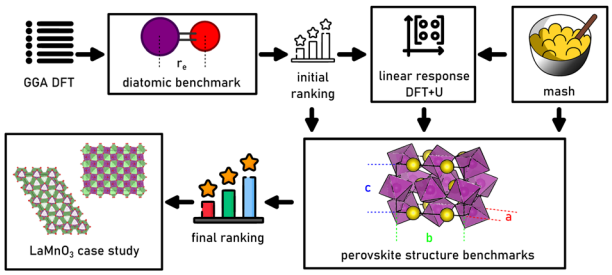

Computational workflows for perovskites: case study for lanthanide manganites

Peter Kraus,* Paolo Raiteri and Julian D. Gale

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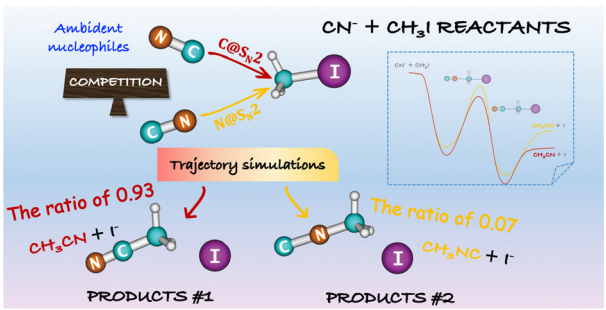

Dynamics of nucleophilic substitution on ambident nucleophiles CN^- and iodomethane: insights into the competition mechanism with neutral isomeric products

Xu Liu, Shiqi Tian, Boxue Pang,* Hui Li and Yang Wu*

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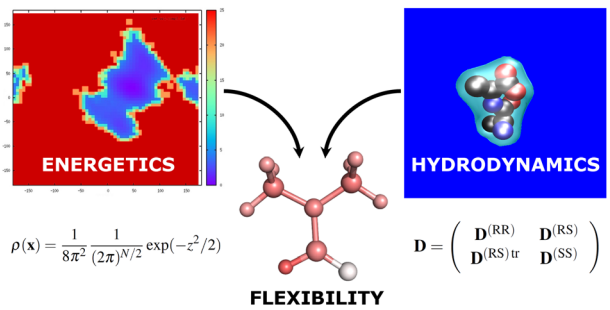

The roto-conformational diffusion tensor as a tool to interpret molecular flexibility

Sergio Rampino, Mirco Zerbetto* and Antonino Polimeno

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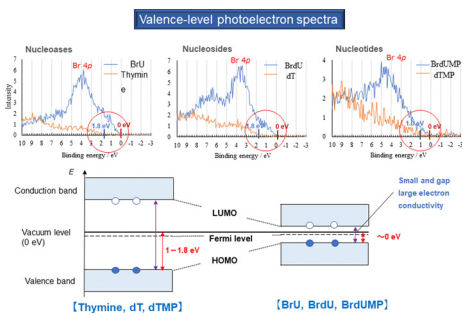

Incorporation of a bromine atom into DNA-related molecules changes their electronic properties

Misaki Hirato, Akinari Yokoya,* Yuji Baba, Seiji Mori, Kentaro Fujii, Shin-ichi Wada, Yudai Izumi and Yoshinori Haga

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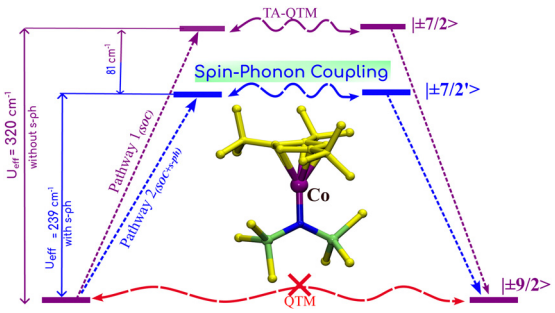

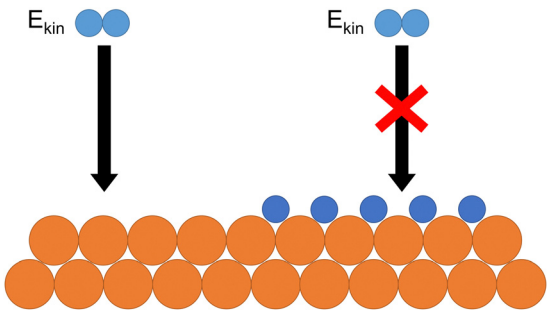

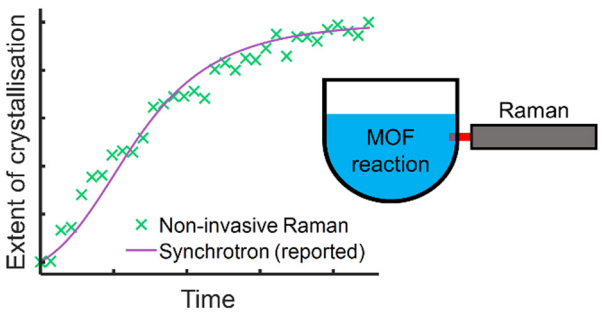

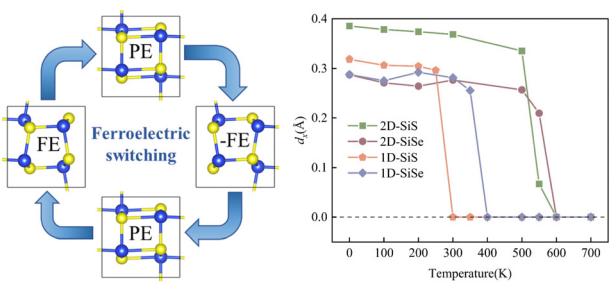

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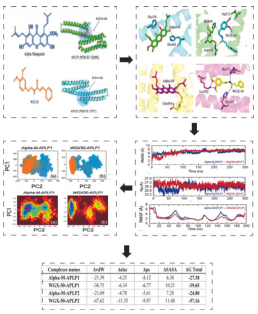
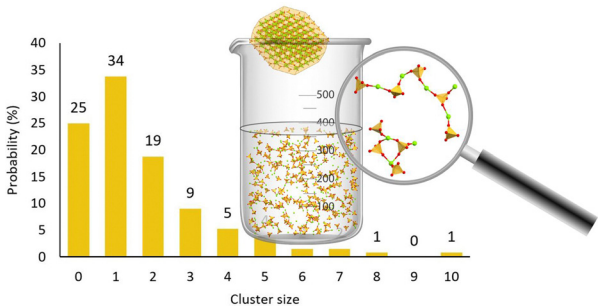


Comparative binding analysis of WGX50 and Alpha-M with APP family proteins APLP1 and APLP2 using structural-dynamics and free energy calculation approaches

Arif Ali, Adan Masood, Abdul Aziz Khan, Feng-Yun Zhu, Muhammad Arslan Rasheed Cheema, Abdus Samad, Abdul Wadood, Abbas Khan, Qiu Yu, Wang Heng,* Daixi Li and Dong-Qing Wei*

14898



A total scattering study of prenucleation structures in saturated aqueous magnesium sulfate – observation of extended clusters

Daniel J. M. Irving, Mark E. Light,* Matilda P. Rhodes, Terence Threlfall and Thomas F. Headen

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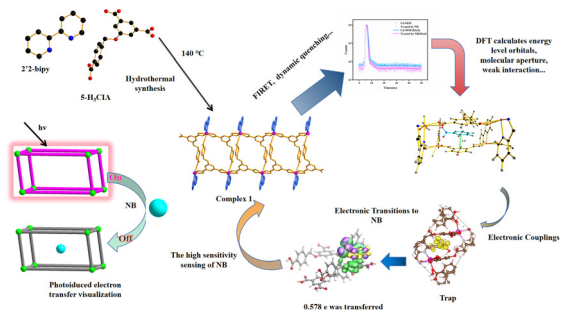

The high fluorescence sensitivity property and quenching mechanism of one-dimensional Cd-HCIA-1 sensor for nitrobenzene

Xiaoming Song, Wenzhuo Dong, Xiufang Hou,* Qingxia Zhao, Zhuangzhuang Zhang and Yixia Ren*

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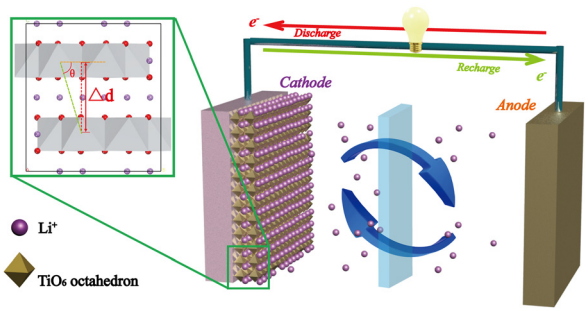

Pressure-induced phase transition toward high symmetry in zero-strain Li_2TiO_3

Wenming Qi, Hadiqa Abdugopur, Wei Xu, Min Gao,* Anwar Hushur* and Hongyan Zhang*

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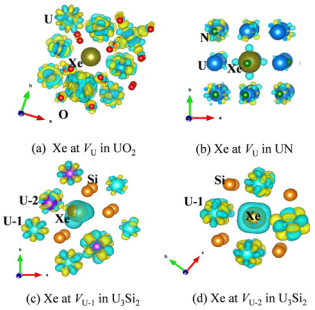
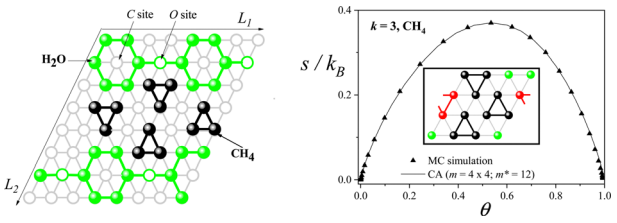
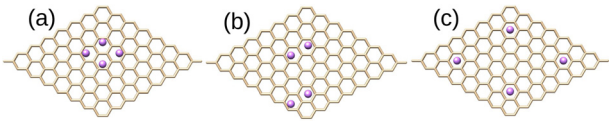
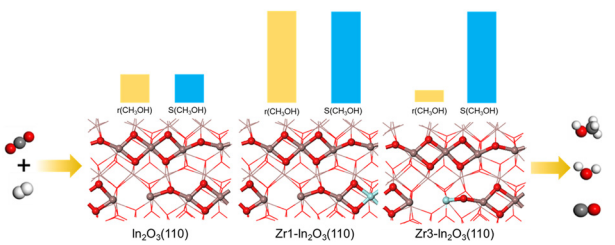


(a) Xe at V_U in UO_2 (b) Xe at V_U in UN

(c) Xe at $V_{U\text{-}1}$ in U_3Si_2 (d) Xe at $V_{U\text{-}2}$ in U_3Si_2







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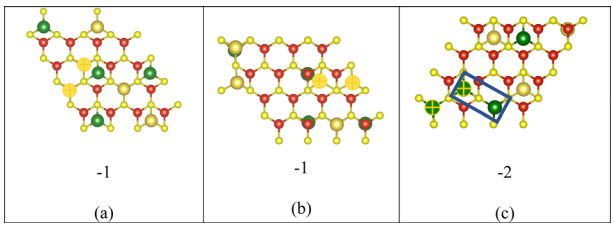

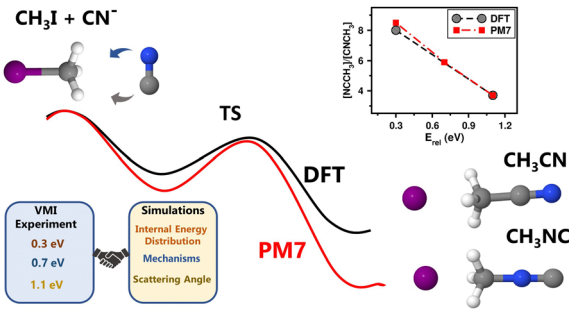

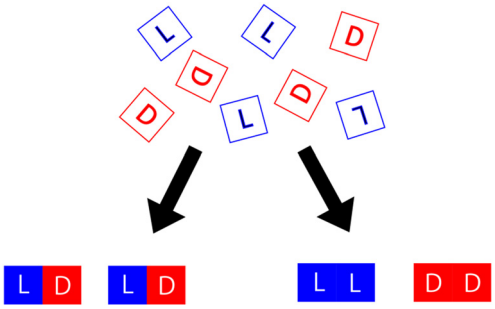

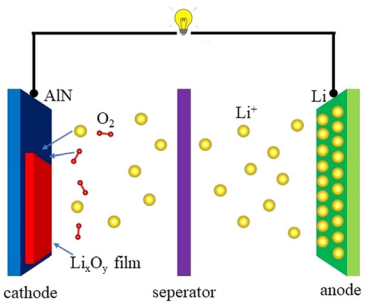

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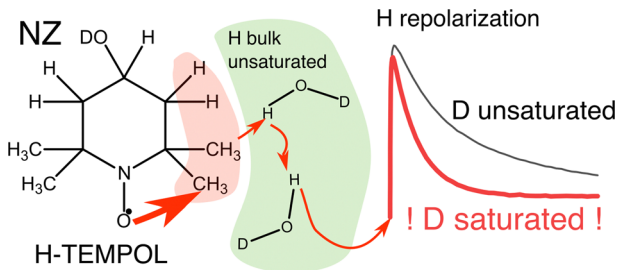

Quantitative analysis of cross-talk in partly deuterated samples of nuclear spins hyperpolarized by dynamic nuclear polarization (DNP) in the thermal mixing regime

Bogdan A. Rodin,* Vineeth Thalakottoor, Mathieu Baudin, Nicolas Birilirakis, Geoffrey Bodenhausen, Alexandra V. Yurkovskaya and Daniel Abergel*

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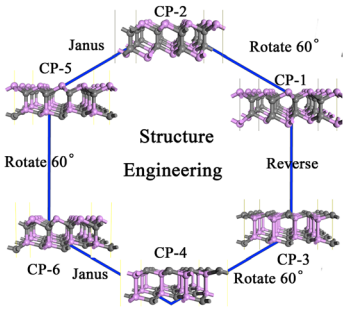

Structure-engineering the stability, electronic, optical and photocatalytic properties of hexagonal C_2P_2 monolayers

Jiahe Lin,* Bofeng Zhang,* Tian Zhang and Xiaowei Chen