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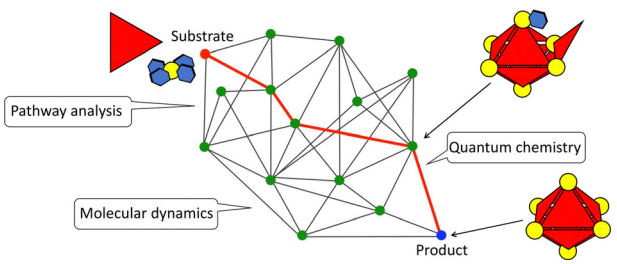
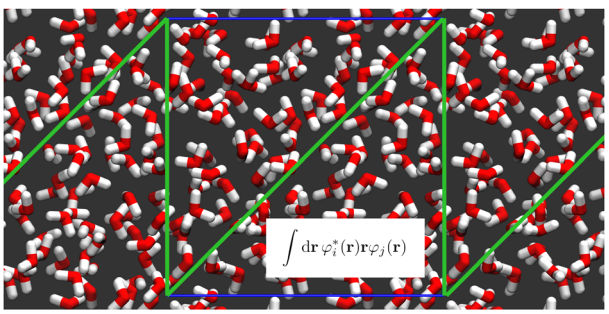
PERSPECTIVES





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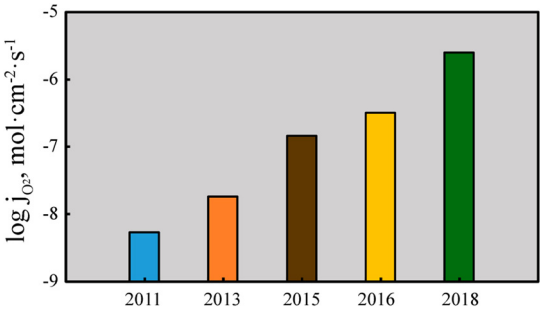

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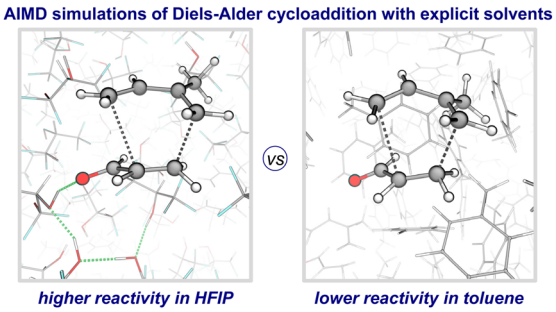

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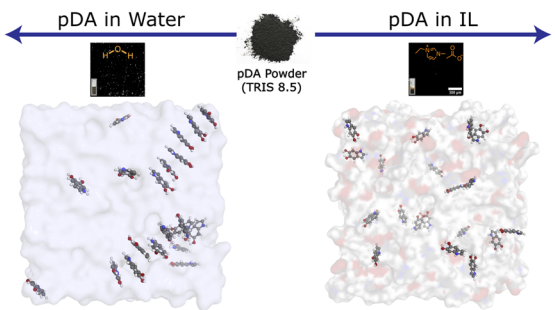

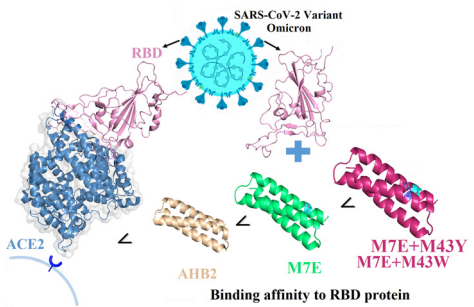

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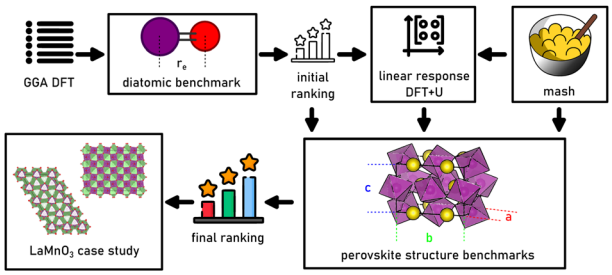

Computational workflows for perovskites: case study for lanthanide manganites

Peter Kraus,* Paolo Raiteri and Julian D. Gale

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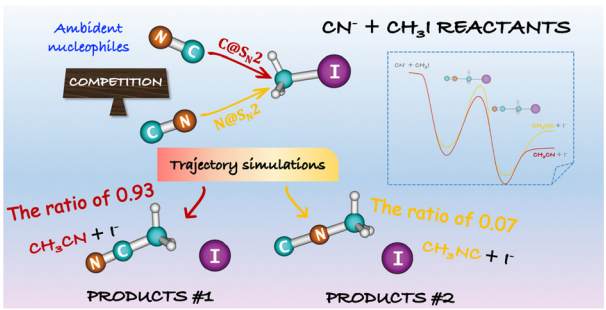

Dynamics of nucleophilic substitution on ambident nucleophiles CN^- and iodomethane: insights into the competition mechanism with neutral isomeric products

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

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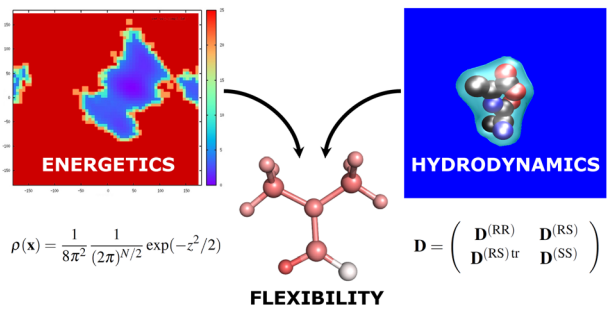

The roto-conformational diffusion tensor as a tool to interpret molecular flexibility

Sergio Rampino, Mirco Zerbetto* and Antonino Polimeno

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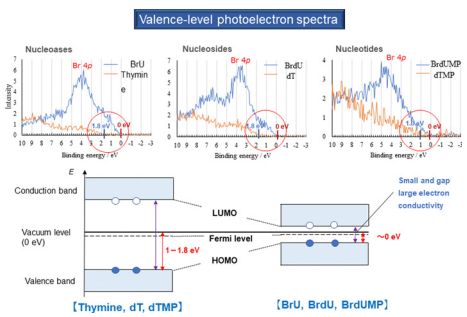

Incorporation of a bromine atom into DNA-related molecules changes their electronic properties

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

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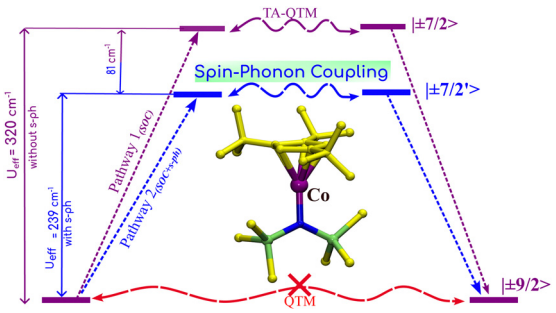

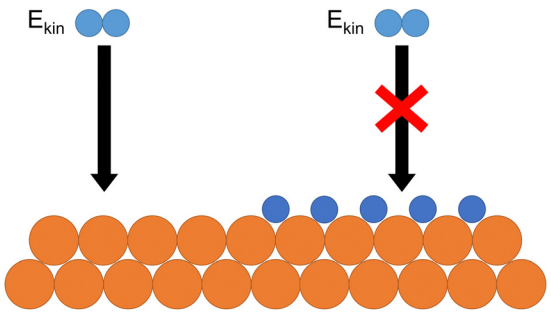

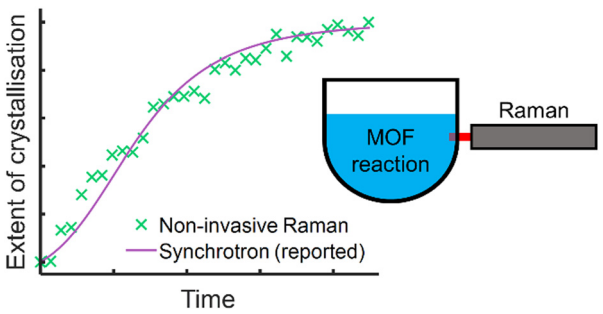

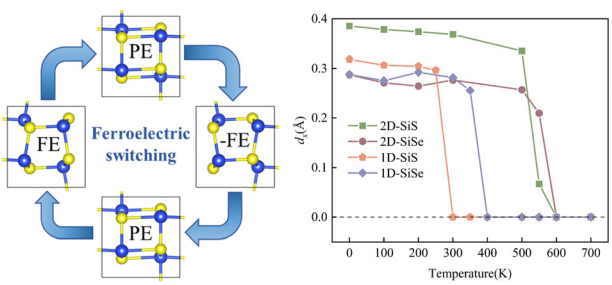

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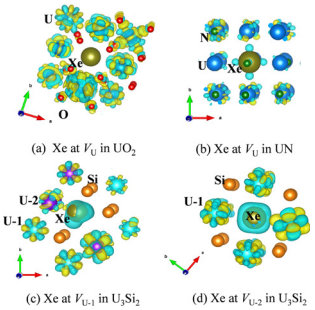

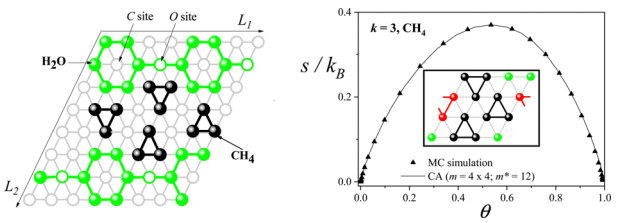

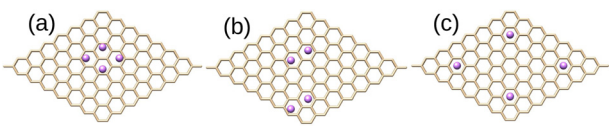

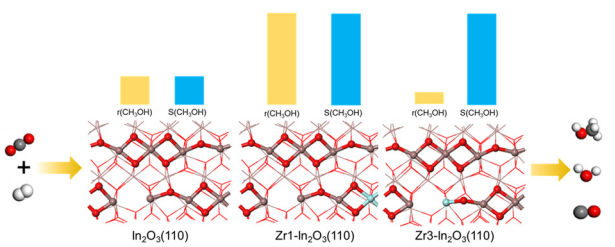

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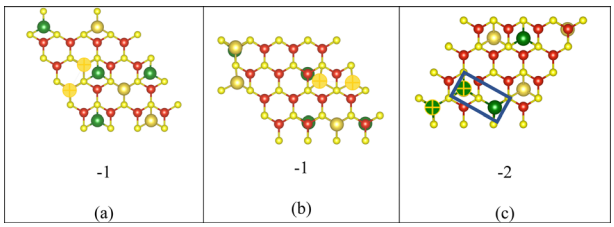

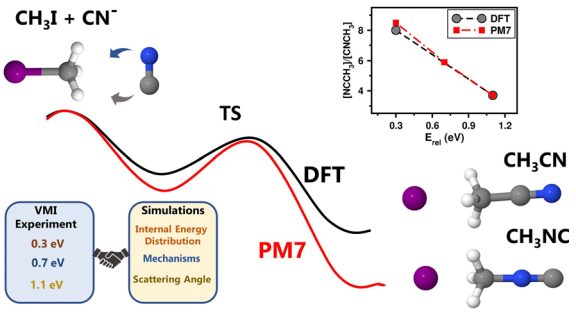

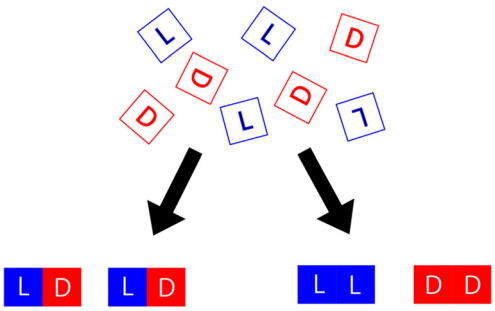

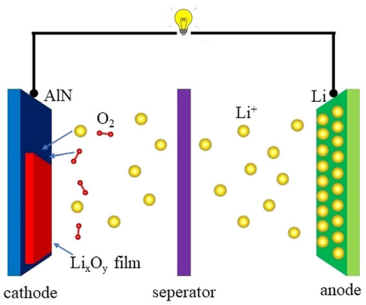

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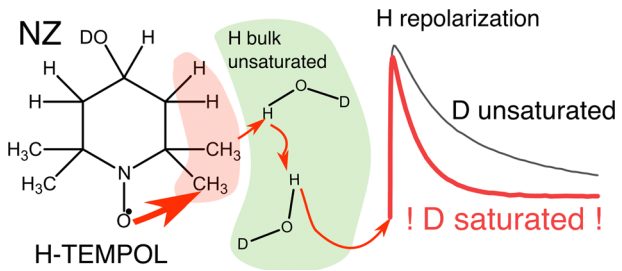
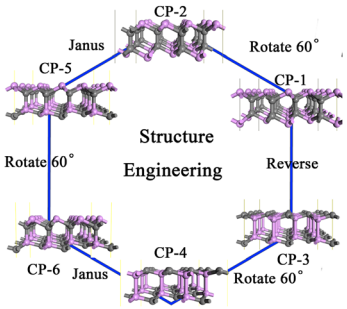


Quantitative analysis of cross-talk in partly deuterated samples of nuclear spins hyperpolarized by dynamic nuclear polarization (DNP) in the thermal mixing regime

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



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

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