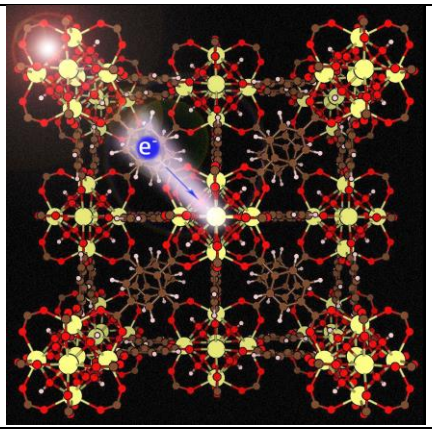
Research Highlight
August 5, 2019

NMGC Theoretical Prediction Confirmed by Experiment

In 2018, work by three NMGC researchers

"Cerium Metal-Organic Framework for Photocatalysis," X.-P. Wu, L. Gagliardi, and D. G. Truhlar, Journal of the American Chemical Society **140**, 7904-7912 (2018). doi.org/10.1021/jacs.8b03613	

predicted that cerium-containing MOFs would be good candidates for visible-response photocatalysis because of charge separation promoted by charge transfer from the ligand to the metal cluster [ligand-to-cluster charge transfer or LCCT]. Now experimentalists at Universidad de Castilla-La Mancha have reported in

"Unravelling Why and to What Extent the Topology of Similar Ce-Based MOFs Conditions their Photodynamic: Relevance to Photocatalysis and Photonics," W. Cabellero-Mancebo, B. Cohen, S. Smolders, D. E. De Vos, and A. Douhal, Advanced Science **2019**, 190120. https://onlinelibrary.wiley.com/doi/10.1002/advs.201901020

that two Ce MOFs show ligand-to-cluster charge transfer resulting in electron and hole generation, "significantly increasing the photocatalytic performance of these materials." They concluded that their observation "shows that Ce-based MOFs are suitable materials for catalysis as they already present LCCT character at the ground state in agreement with the theoretical prediction," that "our experimental results are in full agreement with the theoretical prediction," and that "this will provide more clues to a better design of these materials for photonic applications."

Further theoretical work was reported in

"Metal Doping in Cerium Metal-Organic Frameworks for Visible-Response Water Splitting Photocatalysts," X.-P. Wu, L. Gagliardi, and D. G. Truhlar, Journal of Chemical Physics **150**, 041701/1-8 (2018). doi.org/10.1063/1.5043538

"Photo-Induced Charge Separation and Photoredox Catalysis in Cerium-Based Metal-Organic Frameworks," in *Computational Photocatalysis: Modeling of Photophysics and Photochemistry at Interfaces*, edited by D. Kilin, S. Kilina, and Y. Han (American Chemical Society Symposium Series, Washington, DC), in press.

and

"Computational Studies of Photocatalysis with Metal-Organic Frameworks," X.-P. Wu, I. Choudhuri, and D. G. Truhlar, Energy & Environmental Materials, submitted July 18, 2019.