Poster Presentation

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Probing Chemical Catalysts — How Can Advanced Crystallography Help?

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Crystallography can directly provide ultimate three-dimensional structural information in a way that other science difficult to approach. We will discuss how we have used photocrystallography studies and anomalous scattering analysis to probe chemical catalysts: 1) Photochemical HCl splitting provides an opportunity to store solar energy as a chemical fuel, and is mechanistically simpler than water splitting chemistry. Families of binuclear transition metal complexes have been developed for photochemical HX-splitting but the bottle-neck to development of second generation catalysts is the challenge of halogen elimination chemistry. Current photocrystallography experiments have allowed direct observation of metastable intermediates in the photochemical manifolds of both Rh2 and Pt2 complexes, which has led to the design on new families of halide-bridged Rh2 catalysts for HX splitting. 2) Metal atom substitution within homotrinuclear clusters of Co, Mn, and Fe can have dramatic effects in the local electronic structure, which results in the changes in observed reactivity, substrate binding affinities, and catalytic function. Anomalous scattering measurements are critical for the unambiguous assignment of the trinuclear core composition, which has allowed us to investigate changes in both ensemble electronic structures and reactivity profiles.

[1] *D. C. Powers, S. J. Hwang, B. Anderson, S.-L. Zheng, Y.-S. Chen, D. G. Nocera, in preparation.,* ***[2]*** *T. M. Powers, N. X. Gu, A. R. Fout, A. M. Baldwin, R. H. Sánchez, D. M. Alfonso, Y.-S. Chen, S.-L. Zheng, T. A. Betley, J. Am. Chem. Soc. 2013, 135, 14448−14458.*

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