Computational Approaches to Catalysis: Understanding the Fundamental Principles of Catalysis and Predicting New and more efficient Catalysts.

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The design and realization of catalysts capable of organic oxidation and nitrogen fixation remains a monumental challenge and has occupied some of the most capable investigators for years, and requires in depth understanding of fundamental principles of these vital catalytic processes. First part of my talk addresses in depth hydrocarbon oxidation on multi-component inorganic clusters including metal oxide cluster anions (polyoxometalates or "POMs", such as γ-Keggin and Lindqvist). Second part of my talk describes principles of dinitrogen hydrogenation on multi-component transition metal clusters. I will demonstrate a new and more efficient catalyst capable for dinitrogen hydrogenation and organic oxidation designed based on our theoretical predictions.