Multi-Disciplinary and Collaborative Efforts toward Novel Catalyst and Technology Design

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In this presentation, I will provide an overview of my collaborative efforts that directly relate to the Chemistry Department's missions. I intend to demonstrate that the complexity of the monumental tasks of modern science requires multi-disciplinary and truly collaborative approaches in order to understand the role of each component of a complex system and to elucidate how these components interact and form relationships.

I will briefly present some of latest findings on our ongoing collaborative projects, such as:

(1) **Solar-to-Chemical** conversion (DOE funded, collaborative with C. Hill and T. Lian). Here, I will demonstrate our efforts on the development of all-inorganic transition metal catalysts for water oxidation, designing of novel metal-to-metal charge transfer chromophores, and novel methodology for interfacial electron transfer, and

(2) Transition metal catalyzed **stereoselective CH bond functionalization** (NSF-funded, collaborative with H. Davies, S. Blakey, and other members of the Center for Stereoselective CH functionalization). This talk will elaborate our efforts on understanding the transition metal catalyzed C-H bond alkylation and amination. I will analyze the factors (including nature of catalyst, auxiliary ligands, solvent, base and more) controlling the selectivity of these reactions and make intriguing predictions.

Overall, I intend to show that joint computational-experimental efforts allow us to gain insights into intimate mechanistic details of the reaction and nature of active species. The obtained knowledge is shown to be critical for predicting/designing of new catalysts for water oxidation and selective C-H bond functionalization, as well as for the improvement of reaction efficiency and catalyst TON.