Physical Chemistry Seminar

Tuesday, September 8, 2015 | **11:00 am** | **Room 1315 Chemistry Building**

Probing catalytic reaction intermediates with cryogenic ion vibrational spectroscopy

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Understanding reaction pathways and mechanisms is vitally important for the rational design of catalysts. Toward that end, we developed a method based on mass spectrometry and cryogenic ion vibrational spectroscopy to capture and characterize the reaction complexes formed during homogeneous catalytic reactions. In addition to experimental considerations, this talk will present recent work on model metal hydroxide complexes and the first application of our approach to study catalytic water oxidation. We show that vibrational spectroscopy of the model $M^{2+}OH^{-}$ (M=Mn-Zn) systems can be used to probe the extent of charge transfer between ligand and the metal center and provide a framework for the analysis of more complex spectra. To probe reaction intermediates, we coupled an in-line electrochemical flow cell to our electrospray ionization source, thereby allowing us to controllably reach each step in the catalytic cycle. Using this source, we have successfully isolated and characterized the first few reaction intermediates in water oxidation catalyzed by the single metal center $[Ru(tpy)(bpy)(H_2O)]^{2+}$ catalyst.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315