

# *Ph.D. Dissertation Defense*

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Under the supervision of Professor Etienne Garand

**Friday July 20, 2018 at 2:00 pm in Chemistry Room 8335**



## “Developing Cryogenic Ion Vibrational Spectroscopy Methods for the Characterization of Molecular Interactions”

Molecular interactions play subtle yet important roles in regulating reactivity and three-dimensional structure in both catalytic and biological systems. However, these effects can be difficult to understand with conventional methods due to the simultaneous combination of various forces (dispersion, H-bonding, charge transfer) between multiple species (solute, solvent, surface). Additionally, the study of these types of interactions is often further complicated by the transient nature of such species.

The bulk of my thesis work has involved developing a diverse arsenal of cryogenic ion vibrational spectroscopy techniques for rigorously probing non-bonding interactions at the molecular level. In the first part of my talk, I will discuss an electrochemical flow cell (bottom left) used to prepare delicate intermediates of the  $[\text{Ru}(\text{H}_2\text{O})(\text{bpy})(\text{tpy})]^{2+}$  water oxidation catalyst in addition to the mechanistic role of  $\text{H}_2\text{O}$  in proton-coupled electron transfer in this system. The second part of my talk will focus on a pump-probe laser approach (bottom right) which greatly simplifies analyses of “floppy” molecules that display conformational complexity. Finally, I will present a recently developed clustering technique capable of distinguishing the vibrational signatures of solvent molecules from those of the core ion, providing insight into microsolvation motifs.

