CHEMISTRY COLLOQUIUM

Professor Andrei Tokmakoff

University of Chicago

Department of Chemistry

Wednesday, November 7th, 12:00 pm

140 Hutchison Hall

Lander Auditorium

University of Rochester

Department of Chemistry

Title: "The Ultrafast Structural Dynamics of Protons in Liquid Water"

Abstract: As omnipresent as liquid water is, we still struggle to understand its chemistry at a molecular scale. It is not just a solvent but its rapidly changing network of hydrogen bonds shapes and changes solutes within it. The conceptual and technical challenges of studying such problems are nowhere more apparent than when investigating the transport of an excess proton in water, since it is only distinguishable as an excess charge imbedded in the liquid. Proton transfer in water has long been attributed to a sequential displacement of protons along a chain of hydrogen bonds, but there is little experimental evidence to describe the solvation structure of this charge defect and how it changes in charge transfer. I will describe research being performed to visualize the molecular dynamics of excess protons in liquid water using new techniques in ultrafast 2D IR spectroscopy. Two-dimensional infrared spectroscopy is used to track the time-dependent vibrational frequencies of the aqueous proton complex as it evolves. These results are interpreted with the assistance of spectral modeling based on molecular dynamics simulations. Our results to this point indicate that the proton is best described as a fluctuating complex of a proton strongly bound between a pair water molecules, a structure often referred to as a Zundel complex.

Host: Professor David McCamant • Email: mccamant@chem.rochester.edu