DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
FALL 2018

DATE: THURSDAY, DECEMBER 13, 2018

LOCATION: TIERNAN HALL – 373

TIME: 2:30 PM – 4:00 PM

GUEST SPEAKER

Christopher Rumble
Postdoctoral Scholar
University of Geneva
Department of Physical Chemistry
Geneva, Switzerland

TOPIC

Solute Rotational Dynamics in Ionic Liquids: Experiments and Molecular Dynamics Simulations

ABSTRACT

Steady-state and time-resolved spectroscopies have proven to be invaluable tools for studying chemical and physical processes in solution. Despite their demonstrated utility, all experiments are limited to the physical observables to which they are sensitive and typically report on time and/or ensemble averaged parameters. Such averaging can sometimes wash out molecular level details needed for testing physical models of the experimental system. Molecular dynamics simulations are able to provide exquisitely detailed information inaccessible to experiments, but must first be validated by demonstrating their ability to reproduce key experimental observables. This seminar will present the results of combined experimental/computational studies of solute rotational and conformational dynamics in both dipolar and ionic liquids. These studies serve to illustrate the power of combining modern experimental and computational methods in order to study solution phase processes in greater detail than either experiments or simulations along can provide.

CV

Current Position
August 2017 - Present
Postdoctoral Scholar, University of Geneva, Geneva, CH.
Advisor: Eric Vauthey

Education
April 2017 Doctor of Philosophy, The Pennsylvania State University, University Park, PA.
Department: Chemistry
Advisor: Mark Maroncelli
Thesis title: "Solute Dynamics in Liquid Systems: Experiments and Molecular Dynamics Simulations"
June 2010 Bachelor of Science in Chemistry, The University of Michigan, Ann Arbor, MI.
Research Advisor: James Penner-Hahn

Seminar Series Coordinator:
Yuanwei Zhang