DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
FALL 2019

DATE: WEDNESDAY, DECEMBER 11, 2019

LOCATION: TIERNAN HALL LECTURE 1
TIME: 1:00-2:20PM

GUEST SPEAKER

Dr. Robert Q. Topper
Professor of Chemistry
The Cooper Union for the Advancement of Science and Art
New York, NY

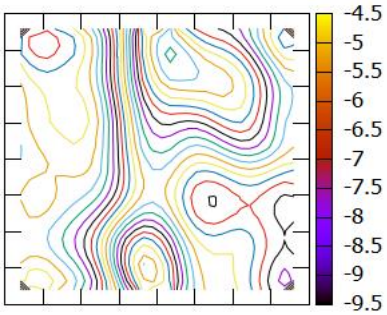
TOPIC

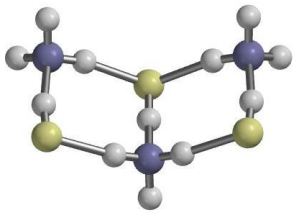
Stochastic Simulation, Quantum Mechanics, and Machine Learning Approaches to Intra-Cluster Proton Transfer and Conformational Diversity

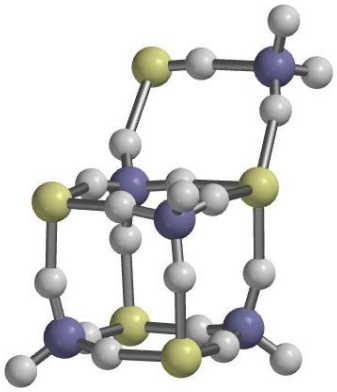
ABSTRACT

The reactions of acids and bases are of fundamental interest and importance throughout all branches of chemistry. These reactions have different pathways in the atmosphere than they do in condensed matter, as the presence of external bodies (even an extra electron) or a polarizable medium is needed to catalyze the transfer of protons when an acid and base encounter one another. In addition to contributing to a better understanding of atmospheric chemistry, the study of these pathways enhances our understanding of intermolecular forces and the thermodynamics of proton transfer. We will describe the use of a rather simple stochastic simulation technique known as "mag-walking" to locate the minimum-energy structures of a variety of ammonium halide clusters followed by DFT, MP2 and CCSD(T) quantum calculations to characterize the thermodynamics of particle growth. The results are compared with thermospray mass spectrometry experiments.

We will also describe collaborative work with the Tuckerman group at NYU, where enhanced sampling molecular dynamics simulations are carried out of polypeptides in solution and solid-solid phase transitions are collected into n-dimensional free energy surfaces. Following the simulations, we use machine learning approaches (including artificial neural networks, Gaussian kernel ridge regressions, and support vector machines) to assimilate the surface. We then can use the trained models for the subsequent prediction of experimental observables.







BIO

Robert Topper is a theoretical physical chemist. His current interests include atmospheric acid-base chemistry, applications of machine learning to problems in molecular biophysics and materials science, and DNA damage caused by metabolism of environmental mutagens. He earned a B.S. in physics and chemistry at Florida State University and a Ph.D. in chemistry at Yale University. His thesis focused on the use of chaos theory to make improvements to transition state theory. He then worked for two years as a postdoctoral researcher at the University of Minnesota, developing quantum Monte Carlo methods for modeling gas-phase chemical reactions in the combustion regime. This was followed by a year at the University of Rhode Island spent modeling order-disorder transitions in solids and nanoparticles before joining the Cooper Union. His work has been published in Physical Review Letters, Journal of Physical Chemistry A, Reviews in Computational Chemistry, Journal of Chemical Physics, and Advances in Chemical Physics.

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