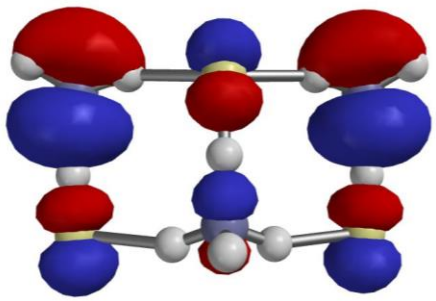
Conference Attendance Report – Prof. Robert Q. Topper, Chemistry

Recently I attended the 2016 Mid-Atlantic Regional Meeting of the American Chemical Society. This meeting celebrated the 125th anniversary of the New York section of the ACS, and took place at the College of Mount Saint Vincent in the Bronx. Two Cooper Union students, George Ho (ChE 2019) and Steven Neuhaus (ChE 2015, M.Eng. 2016) also attended. The students and I benefited from the ability to interact with scientists working on the same types of research questions that we are attempting to solve, as well as to network and interact with students and professionals from the region in chemistry and chemical engineering. In addition to attending various lectures and participating in the discussions, I gave a contributed lecture entitled "*Mag-walking Monte Carlo and density functional theory calculations of interaction energies in ammonium halide clusters* " My coauthors were John Biswakarma (BSE 2014) and Vlad Ciocoi (ChE 2014, M.Eng. 2015). The abstract is attached.

Two other Cooper Union faculty members, Profs. Ruben Savizky and Kevin Kolack, also attended the same conference. Prof. Savisky gave two lectures; one on his research into the historical origins of encaustic art, and one on his work in developing a free MOOC for high school and mature students to learn the foundations of chemistry. Prof. Kolack chaired a session on chemical education.

In our own work, which is currently being prepared for publication, we studied the thermodynamic properties of nanoparticles formed from ammonia and simple acids. The work has some connection to atmospheric process that occur in polluted marine environments here in the United States and elsewhere around the world. One of the remarkable outcomes is that we have been able to identify three distinct kinds of hydrogen bonds within these apparently simple systems. Hydrogen bonds are the forces which hold strands of DNA to one another, stabilize the structures of enzymes, and give water its unique physical properties. An improved understanding of hydrogen bonding is of broad importance. It necessarily leads us closer to being able to computationally model biological systems with reliability and accuracy.



Pictured above: Highest occupied molecular orbital of the ammonium fluoride trimer.
This species exhibits two different types of hydrogen bond, with the outermost pairs linked by traditional hydrogen bonds and the interior pair connected by a proton which is equally shared between the two species.

Mag-walking Monte Carlo and density functional theory calculations of interaction energies in ammonium halide clusters

Robert Q. Topper, John J. Biswakarma, Vlad Ciocoi

Contributions from different intermolecular and interionic forces, as well as variations in bond energies, may produce size-dependent variations in the structures of molecular clusters formed from acid-base chemistry. The growth patterns of ammonium chloride, bromide and fluoride clusters are considered using quantum molecular modeling and "mag-walking" simulated annealing Monte Carlo calculations. Simulated annealing is used to identify local and global minima of the particles. Second order Moller-Plesset (MP2) and M06-2X density functional theory calculations are used to predict the interaction energetics and free energies as a function of size, which correlate well with available mass spectrometric data. Taken together, these three types of systems variously exhibit competition and cooperation between ionic forces, hydrogen bonds, bond energies, and dipole-dipole interactions in an interesting, size-dependent manner. In particular, three different types of hydrogen bonds are predicted in ammonium fluoride clusters.

125th Anniversary
NYACS
NEW YORK SECTION of the AMERICAN CHEMICAL SOCIETY

COLLEGE OF MOUNT SAINT VINCENT

44th Middle Atlantic Regional Meeting

June 9 – June 12, 2016

Chemistry: Past, Present, and Future
New York – A Chemistry State of Mind

College of Mount Saint Vincent
Riverdale, New York

College of Mount Saint Vincent
409, Founder's Hall

Computational/Physical Chemistry

Structure & Thermodynamics in Biological Systems

Cosponsored by COMP, INOR and PHYS‡
Y. Small, *Organizer, Presiding*

10:00 Introductory Remarks.

10:05 362. The role of organized water in mediating ligand-protein interactions. **J.D. Gough**

10:35 363. Multiscale simulations to characterize the blood-brain barrier tight junctions. **S. Nangia**

11:05 364. Molecular interactions of complex biological systems in rare and orphan diseases. **K. Nguyen**, L. Tian, D. Li, M. March, R. Pellegrino, C. Kao, P. Sleiman, H. Hakonarson

11:35 Intermission.

11:50 365. A grand canonical ensemble approach to solution interfaces: Inference of the concentration gradient. **M.N. Kobrak**

12:20 366. Mag-walking Monte Carlo and quantum mechanics predictions of structures and interaction energies of ammonium halide clusters. **R.Q. Topper**, J.J. Biswakarma, V. Ciocoi

12:50 367. Water in dopamine receptors: Using solvation thermodynamics to modify a lead compound for specificity. S. Gadhiya, S. Madapa, T.P. Kurtzman, I.L. Alberts, **S. Ramsey**, N. Pillarsetty, T. Kalidindi, W.W. Harding

1:20 Concluding Remarks.