Pittsburgh ACS Travel Grant Award

Kaye A. Archer

This past spring I attending the ACS national meeting held in Denver, CO under the auspices of the Pittsburgh ACS Chapter. ACS Denver is the first meeting of this scale that I have attended. At first blush, the size of the ACS meeting can be quite intimidating, but that quickly morphed into excitement. Participants and presenters span the spectrum from industry to academia. I especially enjoyed the talks in the computational division dedicated to electronic structure methods for polarizable materials, the poster sessions and literature (textbook) displays.

The highlight of the conference for me though, was the symposium in honor of Dr. George C. Shields, at which I gave a talk. Dr. Shields received the ACS Award for Research at an Undergraduate Institution. Speakers at this symposium were past students and colleagues of Dr. Shields. The most poignant impression I left this symposium with was that engaging undergraduate students in scientific research is paramount. Scientific research spurred their endeavors regardless of the career to which they eventually gravitated.

As a past student of Dr. Shields I spoke on “Mapping the Potential Energy Surface of $H^+(H_2O)_{21}$”. This work was presented on behalf of myself, Tuguldur T. Odbadtakh, Joseph A. Fournier (Yale University), Prof. Kenneth D. Jordan (my current Principal Investigator) and Prof. Mark Johnson (Yale University). This area represents one of the many research interests that is pursued at the Jordan Lab at the University of Pittsburgh. Because of the application to solvation chemistry, atmospheric sciences, etc. this topic garners much interest.

Potential energy surfaces relate energy to structural geometry and offers information about chemical pathways and transition states. Searcy and Fenn (1974) in a gas phase study of protonated water clusters discovered that $H^+(H_2O)_{21}$ is a “magic number” cluster. Due to an interior bound molecule, $H^+(H_2O)_{21}$ is a distorted dodecahedron. The H_3O^+ moiety of the $H^+(H_2O)_{21}$ cluster is now known to be located on the surface of the cluster, this was previously a subject of controversy (Castleman and coworkers1979).

Infrared spectroscopy of the $H^+(H_2O)_{21}$ minima reveal a large redshift of ~500 cm^{-1} of the OH stretch and a blue shift of ~200 cm^{-1} of the umbrella mode associated with H_3O^+ (Johnson and coworkers 2014). Decoding these shifts is a current area of interest in our lab.

I would like to thank Pittsburgh ACS for the opportunity to attend ACS Denver.

Picture taken at the ACS 2015 Award Ceremony. From left to right: Prof. Richard Wallace (Armstrong Atlantic State University), George C. Shields (Dean of Arts and Sciences Bucknell University and recipicent of the ACS 2015 award for research at an undergraduate university, creator and director of Molecular Education and Research Consortium in Undergraduate computational chemistry), Kaye Archer, Prof. William Lynch (Armstrong Atlantic State University, Head of Department of Chemistry and Physics).