

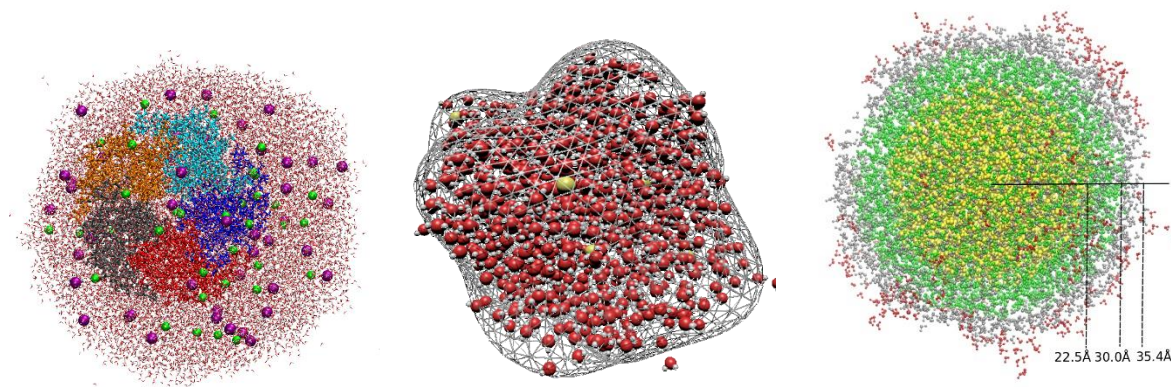
Professor S. Consta

Office: ChB 071

sconstas@uwo.ca

Where do proteins reside in droplets of aerosols?

Charged droplets composed of water, biological macromolecules and multiple ions are ubiquitous in atmospheric and man-made aerosols. Droplets in atmospheric aerosols contain biological molecules because of the presence of viruses, pollen and other biological bodies. Man-made aerosols with proteins and nucleic acids are formed by spraying such as electrospraying. Applications of electrospraying are found in native mass spectrometry. The chemistry within the droplets is very intriguing and different from that of their bulk analogues. In recent innovative experiments that explore the chemical reactivity within electrosprayed droplets in the aerosol phase, certain chemical reactions are accelerated and others are decelerated relative to their bulk analogues. The reasons that lead to the change of reaction rates are still unknown. The location of the proteins in the droplets provides information about the factors that play a role in the distinct reactivity in droplets and in the explanation of mass spectra. In this project the location of proteins in droplets will be studied by molecular dynamics methods and advanced sampling techniques of molecular states for the computation of the potential of mean force. An example of the systems under investigation is shown in the first illustration, where the ring represents the protein complex cholera toxin and the green and purple spheres represent sodium and chloride ions, respectively and the remaining molecules are water molecules. The second illustration shows surface reconstruction of the fluctuating droplet and the last identifies shells with different solvent density in the droplets. The modelling will take place using classical mechanics.



During the course of the project the student(s) will learn state-of-the-art molecular modelling software packages (NAMD and VMD), molecular dynamics and Monte Carlo methods, methods of surface reconstruction (middle illustration). Knowledge of a programming language such as Python, or C++ or C is a desirable skill but not necessary as long as the student is willing to dedicate the time to learn a programming language.

References

1. Kwan, V., Malevanets, A. and Consta, S., 2019. Where do the ions reside in a highly charged droplet?. *The Journal of Physical Chemistry A*, 123(43), pp.9298-9310.
2. Kwan, V. and Consta, S., 2020. Bridging electrostatic properties between nanoscopic and microscopic highly charged droplets. *Chemical Physics Letters*, p.137238.