Professor S. Constas Office: ChB 071 sconstas@uwo.ca

Macroion-droplet interactions in determining the charge states detected in native mass spectrometry

Macroion-droplet interactions play a critical role in many settings such as ionization techniques of samples in mass spectrometry analysis and atmospheric aerosols. The droplets under investigation are composed of a polar solvent, primarily water, a charged macroion and, possibly, buffer ions. We have shown [1] that depending on the charge on the macroion and certain macroscopic properties of the solvent, such as its dielectric constant and surface tension, a droplet may obtain striking conformations such as droplets with extruded tails, ``pearl-necklace'' conformations and multi-point ``star'' shapes. The interactions of nucleic acids and proteins with droplets are shown in the illustrations. The shapes of the droplet containing the macroion influence the charging mechanism of the macroion in a reciprocal manner. The understanding of the macroion-droplet interactions play a central role in explaining the origin and the magnitude of the charge in spectra obtained in electrospray ionization mass spectrometry experiments and in controlling the stability of complexes of nucleic acids and proteins in droplets.





The student will investigate the factors that determine the droplet shapes when they interact with the macroions and the effect of the shapes in the charge state of the macroions.

References:

[1] S. Consta, M. In Oh, M. Sharawy, A. Malevanets ``Macroion-solvent interactions in charged droplets'', Invited feature and cover article by the Journal of Physical Chemistry A, **122**(24), 5239-5250 (2018).