Computational Insight into the Droplet-Ion Interactions

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Charged droplets play a central role in native mass spectrometry, atmospheric aerosols and in serving as micro-reactors for accelerating chemical reactions. The location of ions has often been associated with distinct chemical reactivity in droplets. We present the ion radial distribution and the surface electric field in aqueous charged nanodroplets by using atomistic modeling and analytical theory. The diameter of the droplets that are investigated are in the range of 5 nm to 16 nm and the charge carriers are alkali and halogen ions. We demonstrate the convergence of the scaled ion radial distributions with droplet size. The form of the distribution is supported by a general analytical theory that takes into account a fluctuating droplet interface, an effective screening length of the charges and the finite size of a solvated ion. We compute the electric potential and the electric field near the droplet surface using a multipole expansion. We emphasize the significance of the fluctuations of the normal component of the electric field in ion evaporation via the Born model. Our results assist in understanding the mechanisms of charging of macromolecules in spray-based ionization methods used in native mass spectrometry and the physical chemistry of atmospheric aerosols.