Influence of Polarizability on Ion Distribution Near the Liquid-Vapor Interface of Salt Solutions

Becky Eggimann [S]
Department of Chemistry, Wheaton College, Wheaton, IL, U.S.A.

Ilja Siepmann [C]
Department of Chemistry, University of Minnesota, Minneapolis, MN, U.S.A.

Adiabatic nuclear and electronic sampling Monte Carlo simulations in the Gibbs ensemble are used to explore the ion distribution and solvation structure near the liquid-vapor interface of aqueous solutions. Changes of the charge distributions of the ions and the solvent are represented using fluctuating charge models with or without charge transfer between the species. The solvent is represented by the TIP4P-pol2 model and the solution contains a range of ions that differ in polarizability, but not in size. The simulation data are extensively compared to previous simulations of related systems and, in particular, to a simulation study that investigated the influence of ion size on the interfacial properties.