Modeling of aqueous electrolyte solutions with perturbed-chain statistical associated fluid theory

The vapor pressures and liquid densities of single-salt electrolyte solutions containing NaCl, LiCl, KCl, NaBr, LiBr, KBr, NaI, LiI, KI, Li2SO4, Na2SO4, and K2SO4 were modeled with an equation of state based on perturbed-chain statistical associated fluid theory (PC-SAFT). The PC-SAFT model was extended to charged compounds using a Debye-Hückel term for the electrostatic interactions. Two model parameters for each ion were fitted to experimental pVT and vapor-pressure data. The model is able to excellently reproduce the experimental data up to high salt molalities and even to predict vapor pressures in mixed-salt solutions.