Solvation Structure of Ions in Water

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Molecular dynamics is used to determine the structure of the first salvation shell of several ions and other solutes in water at ambient conditions. The solutes include the ions Li, Na, K, Ca, Cl, nitrate, sulfate, and guanidinium, as well as urea and oxygen. Water is treated using the SPC/E model, and a number of existing models for the ions are considered. The influence of solute concentration on the local structure of water is examined in terms of the second neighbor feature of the oxygen-oxygen pair correlation function. In general, ions rearrange the local structure of water as the concentration is increased, while urea, which is able to readily fit into the water hydrogen bond network, does not. Uncharged, non-polar solutes, such as oxygen, are only sparingly soluble in water and thus have minor influence on the local structure. The distribution of lifetimes of individual water molecules in the first solvation shell is dependent on both the charge (distribution) and the size of the ions. An artificial model, lithium chloride, is used to illustrate this.