Abstract

The dielectric permittivity of salt water decreases on dissolving more salt. For nearly a century, this phenomenon has been explained by invoking saturation in the dielectric response of the solvent water molecules. Herein, we employ an advanced deep neural network (DNN), built using data from density functional theory, to study the dielectric permittivity of sodium chloride solutions. Notably, the decrease in the dielectric permittivity as a function of concentration, computed using the DNN approach, agrees well with experiments. Detailed analysis of the computations reveals that the dominant effect, caused by the intrusion of ionic hydration shells into the solvent hydrogen-bond network, is the disruption of dipolar correlations among water molecules. Accordingly, the observed decrease in the dielectric permittivity is mostly due to increasing suppression of the collective response of solvent waters.