MOLECULAR DYNAMICS SIMULATIONS OF AQUEOUS NaCl SOLUTIONS AT SUPERCRITICAL CONDITIONS: EFFECTS OF ION CONCENTRATION ON THE COLLECTIVE DYNAMIC PROPERTIES

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Supercritical water is an interesting medium for fundamental studies of ionic solutions since the evolution of both structural and dynamic properties can be observed over a wide range of solvent densities [1-3]. In this communication we present the results of a series of computer simulation studies on aqueous NaCl solutions at supercritical conditions. We carried out molecular dynamics simulations along the isotherm T=650K and solvent densities ranging from 500 kgm^{-3} down to 100 kgm^{-3}. The effects of both solvent density and ion concentration on collective dynamic properties have been systematically investigated. To this end, the frequency dependent dielectric constant and conductivity have been calculated. For the sake of comparison results at ambient conditions are also reported.

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