On the relation between the microscopic structure of water and water-alcohol mixtures and density anomaly. Molecular dynamics simulation results.

Edgar Galicia-Andres (Institute of Chemistry, UNAM),
Hector Dominguez (Institute of Material Reasearch, UNAM),
Orest Pizio (Institute of Chemistry, UNAM)

We have investigated temperature dependence of the microscopic structure of the SPC/E and TIP4P-Ew water models in terms of the pair distribution functions, coordination numbers, the average number of hydrogen bonds, the distribution of bonding states of a single molecule as well as the angular distribution of molecules by using the constant pressure molecular dynamics simulations.

The evolution of the structure is put in correspondence with the dependence of water density from high temperatures down to the region of temperatures where the system becomes supercooled. It is shown that the fractions of molecules with three and four bonds determine the maximum density for both models. In the similar manner we investigated water-methanol and water ethanol mixtures of different composition. The SPC/E and the OPLS/UA models are used for this purpose. In addition to the microscopic structure and changes of the shape of the density dependence on temperature, we study the internal energy of the system and the self-diffusion coefficients of species. Moreover, the temperature dependence of the dielectric constant is obtained and analyzed in detail.