Theoretical investigations of the interaction between Single Walled Carbon Nanotubes (SWNT) and water are presented in this article using Molecular Dynamics simulation. Firstly, isolated non-defected and defected SWNT are simulated. Secondly, the effect of chemical functionalization by carboxyl groups on structure-affinity properties of SWNT is discussed at molecular level. Then, SWNT in water is simulated focusing on the SWNT and water interaction as well as electrical properties. It is revealed that increasing numbers of carboxyl groups between SWNT radial deformations in diameter are presented. The diameter decrease of up to 30 per cent of the original size. This deformation process is decreased especially by the insertion of alkyl groups which induces the reduction of radial deformations, especially in those regions most seriously affected. Adsorption of water on SWNT is slower as the polarity of the SWNT decreases. The concentration of water molecules on the surface increased the conductivity.

**Keywords:** SWNT, water, deformations

**References:**


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