Title: Temperature gradient driven transport of water inside a carbon nanotube
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With growing need for micro-nanoscale manipulators and transporters, liquid systems confined in small geometry are of a great interest. An extreme case would be the single walled carbon nanotubes (SWNTs), where the liquid motion is confined in quasi-one-dimensional geometry. In this work, by means of molecular dynamics simulations, we consider the transport of a water cluster which consists of a few hundred molecules in an SWNT with the diameter of about 1.4 nm. Especially, the influence of the non-equilibrium thermal boundary condition on the water cluster is investigated by imposing a longitudinal temperature gradient to the SWNT. Water molecules are modeled with the SPC/E model whereas the carbon-carbon and carbon-water interactions are expressed using the Brenner potential and a simple Lennard-Jones potential, respectively. It is demonstrated that the water cluster is transported with the temperature gradient at an average velocity that is proportional to the temperature gradient. The trend exhibits good correlation with the temperature dependence of the overall potential energy between water and carbon molecules. Together with the comparative case of a water cluster adsorbed on the outer-wall of an SWNT, the molecular dynamics of the transport phenomenon will be discussed.