



سمینار هفتگی گروه  
ماده چگال نرم

# Examination of Water Permeation Through Carbon Nanotubes: A Molecular Dynamics Simulation Study

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Biological water channels have an important role in biological systems. They exist in living cells that the most notable ones are aquaporins, a family of membrane channel proteins, which are abundantly present in nearly all life forms. They have been found in multiple tissues, such as kidney, eye and brain. We have used molecular dynamic simulation to study water permeation in carbon nanotube channels (CNTs). We have investigated both the osmotic and diffusion permeations in three kinds of carbon nanotube channels. We have applied a pressure gradient about (0.12 MPa / 13.4 Å) on the systems for applying a chemical potential difference to explore the osmotic permeation. The diffusion permeation is obtained using no pressure difference. A neutral and two different charge-distributed CNTs have been used to investigate the effect of charge distribution on water permeation. The charge distribution on CNTs is in accordance with the biological channels proposed earlier. We have used these systems as model for biological channels reported recently. We have also investigated the effect of temperature on water permeation in the range of 280 K to 370 K. An interesting result is an abrupt increase in number of diffusion permeation around 340 K. This type of computational investigation can be important in both biology and industrial applications.

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