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EQUILIBRIUM MOLECULAR DYNAMICS MODELING OF DIFFUSSION AND ADSORPTION OF FLUIDS IN ARMCHAIR SINGLE WALLED CARBON-NANOTUBE

Abstract

The aim of this paper is to study adsorption and diffusion of gases and liquids especially Argon and Carbon-dioxide in single walled carbonnanotube at room temeperature using equilibrium molecular dynamic simulation. The simulation domain is developed by the large atomic/molecular massively parallel simulator (LAMMPS). The domain consists of a simulation box of volume 100x100x100 amstrong, having periodic boundary conditions at the x, y and z direction.The adsorption and diffusion of different chirality of carbonnanotubes CNT's are also observed. The MD simulation show that single walled carbonnanotube have affinity to attract carbon dioxide to itself than argon, showing a high adsorption at a certain loading. From this platform we determine at what loading and temperature adsorption and diffusion are likely to occur best in the carbonnanotube. The CNT is assumed to be rigid due to the fact that, flexibility is insignificant and can increase computational time. This study will enable the understanding of storage and filtering of gases in CNTs making it useful in such applications as gasification for jet engines, recycling of urine for usage in the international space station, desalination , air purification, longer space batteries and enhanced oil recovery.