Molecular Dynamics Simulation of Hydrogen Adsorption on Single-wall Carbon Nanotube

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It is desirable to develop a new storage vehicle with high capacity, light mass, and high stability, which may be applicable for portable electronics and moving vehicles. The carbon nanotubes seem to be an ultimate material for this purpose, due to their chemical stability, large surface area, hollowness, and light mass. For these extraordinary properties, carbon nanotube has been proposed as favorable hydrogen storage materials for the automotive industry. In this work, the adsorption of hydrogen molecules onto single-walled carbon nanotubes is studied by molecular dynamics simulation for several temperature and pressure. Also, the effect of chirality for adsorbing hydrogen is investigated by simulation.