Molecular simulation of hydrogen adsorption on carbon nanotube using grand canonical Monte Carlo method

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It is desirable to develop new materials that can store large amounts of hydrogen 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, but there are few experimental results to use commercially. In this work, the adsorption of hydrogen molecules onto carbon nanotubes is studied by grand canonical Monte Carlo simulation for several pressure. Also, the effect of diameter and chirality of carbon nanotube for adsorbing hydrogen is investigated by simulation.