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Understanding the Loading Dependence of Self-Diffusion in Carbon Nanotubes

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Abstract

The influence of loading on the self-diffusion in an isolated single walled carbon nanotube is studied by molecular dynamics simulations. By simulating the carbon nanotube as a flexible framework we demonstrate that the flexibility has a crucial influence on self-diffusion at low loadings [1]. While simulating the nanotube as rigid a remarkable increase of the diffusion coefficient at low loadings is observed [2]. Molecular dynamics simulations of a fully flexible nanotube result in a far less pronounced increase, by a further reduction of the loading the diffusion becomes constant again.

To incorporate the influence of the flexible walls in a simulation of a rigid nanotube, we have introduced a Lowe-Andersen thermostat which works on interface-fluid collisions [1]. The reproduction of the results of a flexible carbon nanotube by a rigid nanotube simulation is excellent. With this approach we simulate the loading dependent self-diffusion in carbon nanotubes. The influence of pore width and temperature on self-diffusion is studied. Furthermore, the influence of adsorption strength is investigated by comparing the self-diffusivities of different components. For small pores, in which the molecules cannot pass each other, single-file diffusion is observed under certain conditions.

References

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