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Ab initio simulation of helium inside carbon nanotubes

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Abstract

In present work we consider the complex behaviour of quantum liquids like liquid He-4 inside carbon nanotubes. Interactions between helium atoms and carbon atoms of the short-length atomistic model and model with periodical boundary conditions of carbon nanotube were studied via ab initio quantum simulations. Effects of geometrical confinement of the tube on the He behaviour inside CNT (13,0) have been explored. Nanotubes with typical average diameter of 10 angstroms are under consideration.

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