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Energy gap engineering of carbon saturated nanowire and investigating ammonia molecule doping effects by the initial calculations

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Abstract

In this paper, the size effects, growth orientation and also, doping by Ammonia molecule (NH₃) on the carbon nanowire properties with the saturated diamond structure by (DNw:H) have been investigated. This study is carried out using DFT theory and Kohn-Sham equation by the self-consistent field (SCF) performed by the local density approximation (LDA). The nanowires morphology is cylindrical with (111) growth orientation and their lateral surface is saturated by hydrogen atoms. The results show that the band gap of these nanowires is smaller than the bulk diamond due to the high surface to volume ratio and the formation surface level. The results of ammonia molecule doping with carbon surface atoms at the saturated diamond nanowire in (100) orientation show the decrease in band gap until the nanowire is converted into an n-type semiconductor.

Keywords: dopant, Ammonia, diamond, cut of energy, growth orientation, self-consistent field, density of states, quantum confinement, band gap, nanowire, density functional theory

For full article, refer to the Persian section