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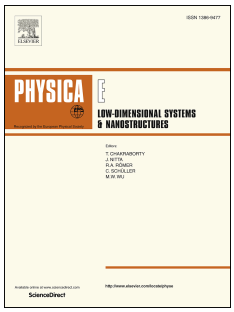

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First principles study of a heavily nitrogen-doped (10,0) carbon nanotube

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Abstract

Using Density functional theory, we studied the effects of adsorption and substitution of nitrogen atoms on structural and electronic properties of (10,0) carbon nanotubes (CNTs). Formation Energy (FE) considerations show that the substitution of nitrogen is more likely to occur than addition. Cohesive Energy (CE) considerations show that both nitrogen-doped CNTs can be achieved and the fabricated structures are all stable. When carbon atoms are substituted by nitrogen atoms, they behave as donors and when the nitrogen atoms are adsorbed on CNTs, they act as acceptors. Nitrogen contamination will turn the semiconducting (10,0) CNT into a metallic nanostructure, except for a special situation when the two nitrogen atoms are in chemically bonded to each other in which the resulting structure acts as a narrow gap semiconductor.

Keywords: Density functional theory, Heavily nitrogen-doped carbon nanotubes, Band Structure, Formation Energy, Cohesive Energy, Stability

1. Introduction

Carbon nanotubes (CNTs) are one of carbon allotropes discovered 4 decades earlier[1]. Single-walled CNTs (SWCNTs) are nanostructures that could be defined by rolling a grapheme sheet into a cylinder[2, 3]. These nanomaterials have surfaces with a thickness of a carbon atom radius. While graphene has a wide surface, SWCNTs have smaller surface and hence CNTs could be used in situations where the wide surface of graphene is not suitable. Although CNTs do not have an effective surface, one can fabricate more useful nanomaterials-based devices compared to graphene, using an array of functionalized CNTs[4, 5]. Due to their various interesting physical properties such as plastic transport, excellent mechanical properties, good capability for sensing toxic gases and …, CNTs have been considered by many researchers[2, 6-8]. Regarding other nanotubes (NTs), CNTs were discovered earlier meaning that production of CNTs are simpler than other kinds of NTs. Investigations show that electronic properties of CNTs depend on their chirality: they can be gapless or a semiconductor with gaps between ranging from 0 to

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