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Study of Structural and Electronic Properties of Doped Arm Chair Single-Walled Carbon Nanotubes

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Abstract

Structural and electronic properties of endohedrally doped armchair single-wall carbon nanotubes (SWCNTs) with a chain of six atoms of Ag and Cu have been studied using ab-initio density functional theory. We investigate the binding energy/atom, ionization potential, electron Affinity and Homo-Lumo gap of doped armchair SWNTs from (4,4) to (6,6) with two ends open. BE/atom is maximum for (5, 5) doped armchair carbon nanotube; suggest that it is more stable than (4, 4) and (6, 6) doped tubes. Whereas ionization potential of Ag doped tubes is more and electron affinity is less with respect to of Cu doped tubes showing that Ag doped tubes are less reactive than Cu doped tubes. Homo- Lumo gap of doped arm chair tubes decreases exponentially with the increase in diameter of the tubes. This shows that confinement induce a strong effect on electronic properties of doped tubes. These combined systems can be used for future Nano electronics. The ab–initio calculations were performed with SIESTA code using generalized gradient approximation (GGA).

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Keywords:Density functional theory; SIESTA; Single-walled armchair carbon nanotubes; HOMO-LUMO gap.

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1. Introduction

Carbon nanotubes (CNTs) have exceptionally high tensile strength, high resilience and semiconductor behavior, high current carrying capacity and high thermal conductivity [1-3]. CNTs can be classified with respect to its structure by means of the roll up or the chirality vector. The chirality vector defines the roll up angle and the circumference of the CNTs. On the basis of classification based on chirality vector there exists three kinds of CNTs: armchair (n, n), chiral (n, m) 0<|m|<n and zigzag (n, 0) [4-6]. Carbon nanotubes (CNTs) have attracted considerable attention owing to their intriguing properties and potential applications to many fields [7-18]. It has been demonstrated that they also possess remarkable mechanical properties and interesting electrical transport behaviors enabling their use in nanoelectronic devices, energy storage, field emission displays, chemical and biological sensors, and other technological fields [19-21]. Single- walled carbon nanotubes (SWCNTs) filled with metals have applications in high- density magnetic data storage devices, nanoscale switches, air stable p-n junction diodes, etc. [32-36].Since CNTs are hollow cylindrical structures [1], they could serve as containers of atoms and small molecules [22-24]. In this regard they could also be used for hydrogen [25]. In particular, CNTs filled with metals represent a fascinating new material and are an effective route to exploit one dimensional nanocables with various uses. These CNTs covering metal nanowires have a significant potential application in data storage nanotechnology due to their small size. In addition, the carbon shells provide an effective barrier against oxidation and ensure long – term stability of the metal core [26-29].

The introduction of metal atoms into single-walled carbon nanotubes cavities may result in the creation of principally new type of functional nanostructures whose physical properties depend on the properties of pristine nanotubes and inserted nanoparticles. In particular, it was shown theoretically that the introduction of such metals as silver and copper in SWCNT channels can lead to an increase of the electronic density on the nanotube walls and the transition to a metallic state [37-39]. For filling SWCNTs with metals, a method from a gas phase is usually employed [40]. Recently CNTs filled with copper have been prepared by various experimental methods [30, 31], but few studies on energetics and electronic structures of copper atomic chains bound in CNTs have been reported in detail. In the present work the binding energies and electronic structures of a linear Cu atomic chain of six Cu Atoms and six Ag atoms in 4,4 armchair, 5,5 armchair and 6,6 arm chair carbon nanotubes have been investigated in detail. All the arm chair carbon nanotubes have same length and different diameters.

The paper is organized as follows: the computational details are discussed in Section 2, results and discussion in section 3 and conclusions in section 4.

2. Computational Detail

We have used the Spanish initiative for electronic simulation with thousands of atoms (SIESTA) computational code. This is based on the numerical atomic orbital density functional theory method [41-43]. The calculations are carried out using the generalized gradient approximation (GGA) that implements Perdew, Zunger and Ernzerhof (PBE) exchange correction. Core electrons are replaced by non-local, nonconservingpeudopotentials factorized in the kleinman-Bylander form [44].

The valence electrons are described using linear combination of numerical pseudo atomic orbitals of the Sankey – Niklewski type [45], but generalized for multiple-ξ and polarization functions. In this work we have used a split valence double ξ polarized basis set (DZP). The cut off is fixed by the “energy shift” parameter = 0.15eV (the change in the eigen state of the free atom due to confinement). For self-consistent calculation of Hamitonian matrix elements, the charge density is replaced by a real space grid of cut off energy 200 Ry. The structures are obtained by minimization of total energy using Hellmann- Feynman forces including Pulay–like corrections.