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# Coverage dependent magnetic properties of Co chain-coated carbon nanotube

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**Abstract**

Magnetic properties of Co chain-coated carbon nanotube (CNT) were investigated using a first-principles calculation. Binding energy between Co chain and CNT increased with the coverage ratio, and the adsorption of Co chains on CNT enhanced the conductance channel. Total magnetic moment of Co chains coated on CNT increased with the coverage ratio, while the magnetic moment per Co atom decreased due to spin flip of majority spin states in Co atoms. Spin polarization at the Fermi level of the Co chains was calculated to converge to that of bulk fcc Co.


*Keywords:* Nanotube; Nanoparticle; Density functional theory; Magnetism

## 1. Introduction

Metal-coated carbon nanotubes (CNTs) have attracted great scientific and technological interest because they are templates for obtaining the continuous ultrathin nanowires, nanomagnets, and new spin polarized electron sources [1–3]. The one-dimensional structure of CNTs provides platforms for physical processes and chemical reactions [1]. Fabrication of nanoscale devices based on CNTs includes filling metal into hollow channel of CNTs, encapsulating nanowires, coating of metals on the sidewall of CNTs, and forming ultrathin nanowire on CNT template [4].

Zhang et al. [5] synthesized Ti, Ni, and Pd continuous nanowires by coating the metal atoms on CNT using electron-beam deposition. The Au, Al, and Fe coated CNT do not form continuous nanowires but discrete particles [1]. This is because a weak interaction between the metals and the sidewall of CNT leads to disconnected coating on CNT. However, the Au, Pd, Fe, Al, and Pb metals were fabricated to form continuous nanowires by evaporating them on Ti-buffered CNT [5]. A buffer layer of Ti helps the metal atoms to stick on the CNT substrate. Deng et al. [2] coated Co metal on Ti-buffered CNT to make a magnetic force microscopy (MFM) tip. The CNT tip is coated by 7 nm Co layer to magnetize the tip, and high resolution by the tip depends on the thickness of metal coating. However, the amount of coated magnetic materials has not been optimized. The understanding of coverage dependent magnetic properties and stability between Co and CNT is needed for the high resolution of MFM–CNT tip coated by Co metal.

In a theoretical study [6], magnetic moment and spin polarization of Co-coated (9,0) CNT with a coverage ratio of 0.5 (Co/C ratio) are found to be $1.21\mu_B$/atom and 84%, respectively. The spin polarization is 20% higher than that of bulk hcp Co, since the conduction electrons are delocalized by hybridization between the C-p and the Co-d-orbital. For magnetic properties of Ti-coated CNT, it was found by ab initio calculations that the magnetic moment and spin polarization depend strongly on geometry,

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amount of Ti coverage, and elastic deformation by Ti-coating [7]. The calculated magnetic moment decreases when the coverage ratio becomes larger than 0.5, while the conduction channel of majority and minority spin states increases. Spin polarization at the Fermi level is enhanced with the increasing axial strain.

In this paper, we studied the magnetic properties of Co chains coated on CNT for three coverage ratio. Spin polarized conduction channel, magnetic moment, and spin polarization at the Fermi level of Co-coated CNT are calculated using the ab initio SIESTA code [8].

## 2. Computational details

We investigated the coverage dependent magnetic properties of Co-coated (4,4) CNT. We performed self-consistent calculation to solve the Kohn–Sham equations [9] with the pseudoatomic orbitals proposed by Sankey and Niklewski [10]. We used a double-zeta basis set with polarization functions [11]. For the exchange–correlation potential, the generalized gradient approximation (GGA) is used [12] and the standard norm conserving Troullier–Martins pseudopotentials is adopted [13]. We have used 14 Monkhorst–Pack $k$-points for the Brillouin zone integration along the tube axis. The geometry is optimized until the atomic force is less than 0.04 eV/Å using the conjugate gradient method.

The atop site was reported to be the most stable site for a single Co atom outside the (4,4) CNT [3]. However, when a linear Co chain is adsorbed on CNT, a bridge site between two C atoms is most favorable energetically [14]. Thus we considered that Co chains are directly adsorbed on the sidewall of CNT. For the calculation, we adopted supercell approximation with periodic boundary condition. We took 32 carbon atoms with a cell height in the growth direction of 4.919Å and a lateral separation of 20Å between CNT centers which prevents any interaction between tubes.

## 3. Results and discussion

We considered three systems of Co-coated CNTs with the coverage ratio of 0.063, 0.125, and 0.25, as shown in Fig. 1. The binding energy, amount of charge transfer, exchange splitting, magnetic moment, and spin polarization are presented in Table 1. The binding energy is defined by

$$E_b = (-E_{CNT+Co} + E_{CNT} + nE_{Co})/n, \quad (1)$$

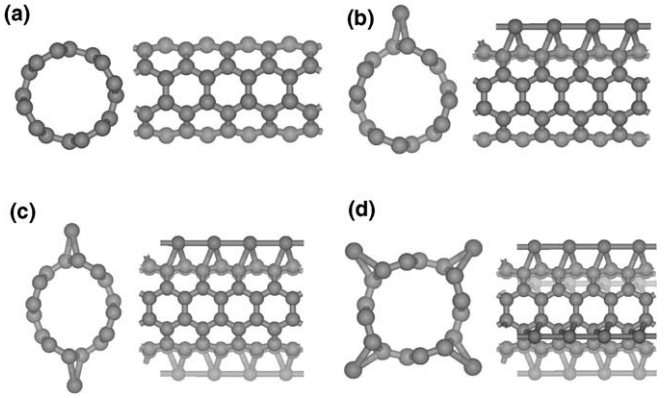


Fig. 1. (a) Pure (4,4) CNT. Co-coated (4,4) CNT with the coverage ratio of (b) 0.063, (c) 0.125, and (d) 0.25.

where $E_{CNT}$ and $E_{Co}$ are the energies of isolated CNT and Co chain, respectively, and $E_{CNT+Co}$ is the total energy of combined system with $n$Co chains. The binding energy is defined as the adsorption energy of a Co chain coated on CNT. The exchange splitting can be calculated as the difference of the energies at which the majority and minority spin DOS peaks are located. The spin polarization, SP, is obtained through the ratio of difference and sum of DOS at the Fermi level as $SP = (\rho_\uparrow - \rho_\downarrow)/(\rho_\uparrow + \rho_\downarrow)$, where $\rho_\uparrow$ ($\rho_\downarrow$) represents the total DOS of majority (minority) spin at the Fermi level.

The Co-coated (4,4) CNT with the coverage of 0.063 has the Co–C bond length of 2.06 Å. We found the binding energy increased with the coverage ratio. The binding energy

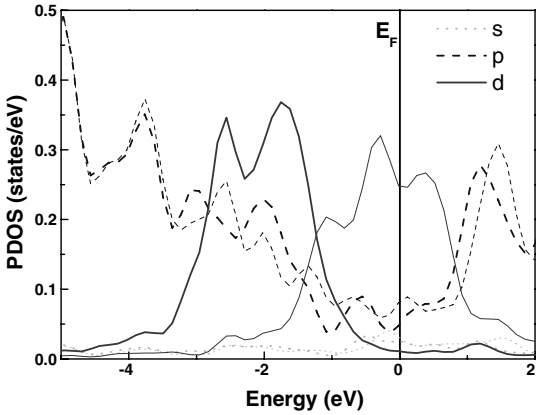


Fig. 2. Orbital-decomposed PDOS of a Co-coated (4,4) CNT. The dotted, dashed, and solid lines indicate s-, p-, and d-orbital PDOS, respectively. The thick (thin) line denotes the majority (minority) spin PDOS.

Table 1
Binding energy ($E_b$), amount of overall charge transfer from Co chain to CNT ($\Delta\varepsilon$) per Co atom, exchange splitting at the top of d-PDOS ($E_x$), magnetic moment ($\mu$), and spin polarization (SP) for Co-coated (4,4) CNT

| Coverage | $E_b$ (eV) | $\Delta\varepsilon$ (e) | $E_x$ (eV) | $\mu$ ($\mu_B$/atom) | SP (%) |
|---|---|---|---|---|---|
| 0.063 | 1.23 | 0.067 | 2.27 | 1.91 | 61 |
| 0.125 | 1.29 | 0.064 | 2.34 | 1.73 | 65 |
| 0.25 | 1.30 | 0.052 | 2.40 | 1.71 | 65 |