A Theoretical investigation of magnetic, optical and electron-conduction properties of transition metal nanowires

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Abstract - Three-strands helical shell structures of M_{19} (M=Fe, Co, and Ni) nanowires (NWs) are obtained by means of the molecular dynamics (MD) method (Figure 1). The magnetic, optical and electrical transport properties of NWs are investigated. The electronic transport properties of optimized NWs sandwiched between two gold electrodes are investigated using non-equilibrium Green´s function (NEGF) formalism. The DOS, transmission functions (T-E), current-voltage (I-V) characteristics, and conductance spectra (G-V) were analyzed in detail. The optical properties of NWs were studied using density functional theory (DFT) calculations. The variation curves of reflectivity $R(\omega)$, absorption $I(\omega)$, refractive index $n(\omega)$, dielectric function $\varepsilon(\omega)$, conductivity $\sigma(\omega)$ and Loss function $L(\omega)$ as the frequency were discussed. The magnetic properties were investigated within non-spin-polarized (NSP) and spin-polarized (SP) ab initio calculation. The density of states (DOS) and electron density difference (Figure 2) were also obtained.

Because of its ability to miniaturize electronic circuits and maximize perpendicular magnetic memorial density further, nanowires (NWs) has been paid most attention over the past few decades, the remarkable achievements have been made specially in microelectronics, optical and spintronics [1]. As one of the most important candidates of the design of electronic, optical and magnetic devices, NWs are being extensively investigated; due to not only their exotic and stable atomic structure, but also their superior performance. Recently, a great deal of experimental work on reproducible synthesis has been performed to seek NWs with controllable electronic, optical and magnetic properties; and then suspended monatomic chains, strands, and helical structures have been realized experimentally [2]. Moreover, many theoretical studies of ultra-thin NWs have been performed using atomistic simulations, and some straight line uniform and helical multi-shell ultra-thin NWs have been obtained [3].

Metal NWs have recently attracted considerable attention due to displaying interesting quantum phenomena that may be exploited to generate novel electronic and magnetic recording devices. Metallic NWs have been fabricated and studied by various methods such as STM/MCBJ and STM/HRTEM. Especially, ferromagnetic metallic NWs have attracted a great interest because of their applications to new nanodevices, spin polarized electron sources with high magnetoresistance values, and high density perpendicular magnetic recording media with high coercivity. Thus Fe, Co and Ni NWs have been widely investigated both experimentally and theoretically.

In this work, we use density function theory (DFT) to obtain optimized three stands helical M_{19} (M=Fe, Co and Ni) NWs, and the electronic transport, optical and magnetic properties of these NWs are studied. Our studies show that the conductance fluctuation of the Co_{19} NWs was more symmetric than those of Fe_{19} and Ni_{19} NWs, thus Co_{19} NWs have tremendous potential in the development of nanoelectronic devices. Moreover, Co_{19} NWs have larger reflectivity, absorption, conductivity, loss function and lower refractive index, dielectric function, and can be used as nanoscale optical materials. In particular, we suggest that Co_{19} NWs with high spin polarization could be useful as spin-valve in spin-dependent transport nanodevices.

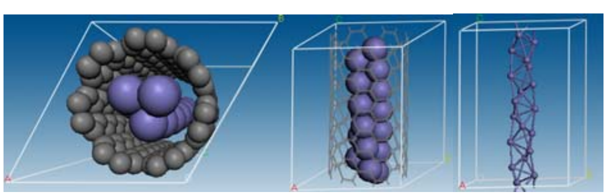

Figure. 1. Images of the M_{19}@(7,7,7)SWCNT and M_{19} (M=Fe, Co and Ni) nanowire.

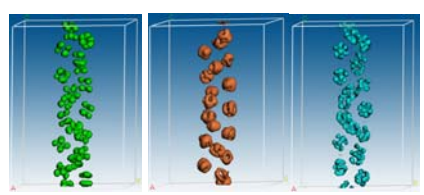

Figure 2. Spin-polarized electron density difference plot (Green, orange and cyan denote density of Fe, Co and Ni, respectively

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