Atomic and Electronic Properties of Ni Filament Encapsulated Inside Single-walled Carbon Nanotubes of Different Chiralities

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Introduction

Nanotubes and atomic nanochains are two of the most important one dimensional nanostructures which have been fabricated and studied in recent years for their remarkable physical, chemical and mechanical properties and thus the great potential applications in nanodevices. In this study, we consider monoatomic chains of nickel atoms encapsulated into single-walled carbon nanotubes (CNTs) of zigzag-type (*n*,0) and armchair-type (*n*,*n*) chiralities with varied *n* indices. We determine the optimal size of the CNT for encapsulating a single atomic wire, as well as the most stable atomic arrangement adopted by the wire. We predict that encapsulation of Ni filament inside CNTs is a way for reliable creation of stable conductive quasi-one-dimensional hybrid nanostructures, even if both the nanotube and the wire are insulators.

Computational details

We have performed *ab initio* LCAO calculations using the hybrid Kohn-Sham exchange-correlation functional PBE as implemented in *CRYSTAL-09* code.

All electron basis sets have been used: Ni – 8-64111(41d)G , C – 6-311(11d)G. Irreducible Brillouin zone has been sampled using 8x1x1 Pack-Monkhorst mesh or 6 *k*-points per segment.

Performing large-scale calculations within the Density Functional Theory (DFT) we obtain the equilibrium geometry of single Ni filament inside CNTs.

Results

Structure	E^f (eV/atom)	d_{Ni-Ni} (Å)	S_{Ni-Ni} (%)	l_{Ni-C} (Å)	l_{C-C} (Å)	P_{Ni-Ni} (me)	P_{Ni-C} (me)	M_{Ni}, (μ_B)
Ni/CNT (6,6)	-0.1001	2.463	+9.22	4.112	1.426	512	2	1.270
Ni/CNT (5,5)	-0.1269	2.464	+9.27	3.439	1.428	472	4	1.119
Ni/CNT (12,0)	-0.0819	2.133	-5.41	4.784	1.423	670	2	1.211
Ni/CNT (11,0)	-0.0896	2.130	-5.54	4.358	1.422	684	2	1.210
Ni/CNT (10,0)	-0.1027	2.138	-5.19	3.973	1.422	676	0	1.263

Table 1. Energy of formation, E^f; distance between neighbored Ni atoms in filament, d_{Ni-Ni}, change in Ni-Ni distance in Ni/CNT filament relative to vacuum position, S_{Ni-Ni}, Ni-C bond length, l_{Ni-C}, C-C bond length, l_{C-C}; Ni-Ni bond population, P_{Ni-Ni}; Ni-C bond population, P_{Ni-C}, and magnetic moments on Ni atoms, M_{Ni} as calculated by means of LCAO-DFT approach.

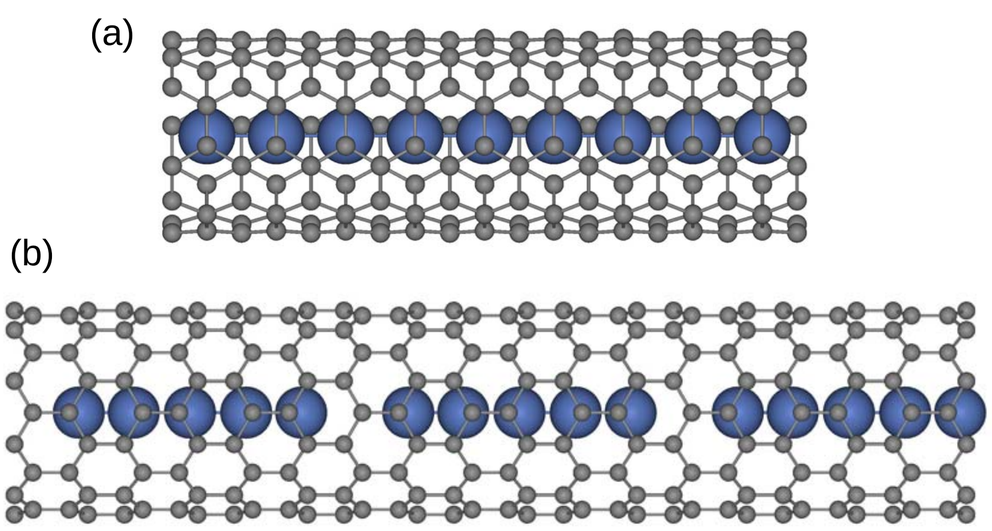

Fig.1. LCAO-DFT calculated equilibrium structures of (a) Ni filament inside CNT (5,5); (b) Ni filament inside CNT (10,0).

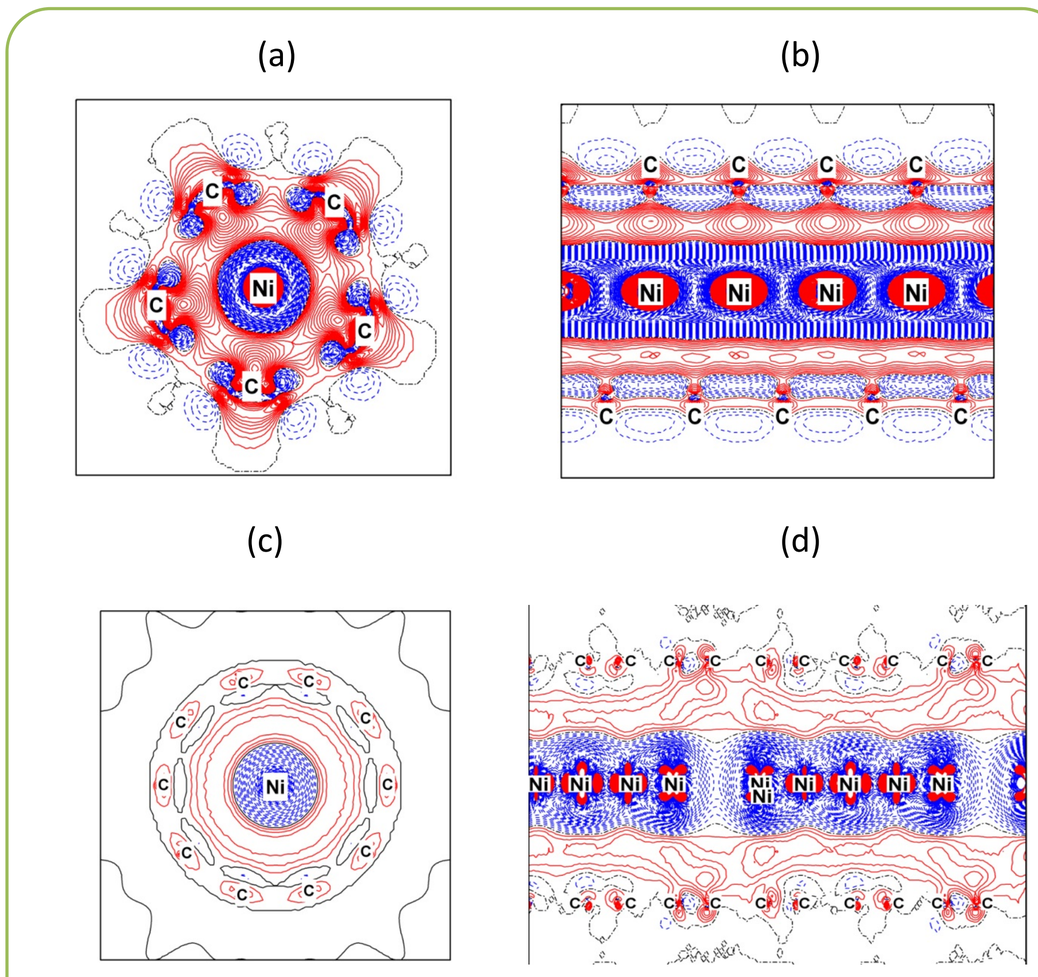

Fig. 2. Difference electronic charge density maps as calculated for (a) Ni/CNT(5,5) front view, (b) Ni/CNT(5,5) side view, (c) Ni/CNT(10,0) front view, and (d) Ni/CNT(10,0) side view.

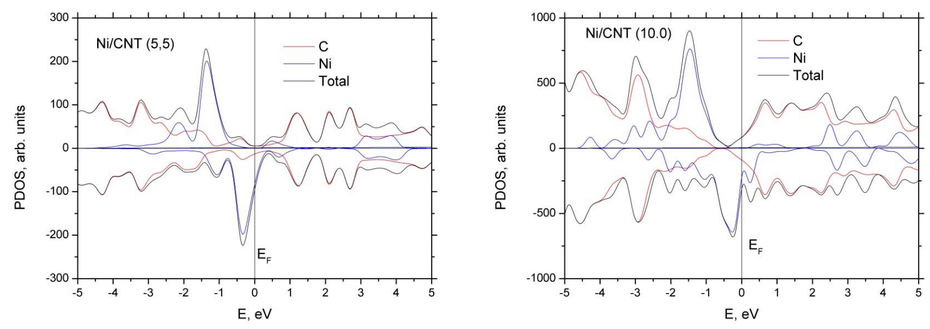

Fig. 3 Total and Projected Densities of State (DOS) as calculated for Ni/CNT (5,5) (a) and Ni/CNT (10,0) (b) nanostructures.

Summary

Ni-*ac*-CNTs are found to be a more stable structure, with a stronger interatomic Ni-C bonding than Ni-*zz*-CNTs, due to smaller energy of formation. The most preferable for Ni filament insertion are found to be CNT(5,5) and CNT(10,0).

In all the cases, Ni filament preserves a ferromagnetic ground state. Calculated magnetic moment of Ni filament is twice larger than in the Ni bulk (0.62 μ_B).

Ni filament tends to be clustered if placed inside CNT (n,0).

Our calculations show that CNTs with Ni filament exhibit metallic behavior, even if pristine nanotube is semiconductor (*i.e.*, *zz*-type).

FM&NT 2012

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Eiropas Sociālā fonda projekts
"Datorzinātnes pielietojumi un tās saiknes ar kvantu fiziku"
Nr.2009/0216/1DP/1.1.1.2.0/09/APIA/VIAA/044