Stability, electronic structure and conductivity of monoatomic Mo wires inside carbon nanotubes

A. Vega,[1] A. García-Fuente,[1] V. M. García-Suárez,[2] J. Ferrer[2]

[1]Departamento de Física Teórica, Atómica y Óptica. Universidad de Valladolid, Spain
[2]Departamento de Física. Universidad de Oviedo, Spain
vega@phenix.fam.cie.uva.es

We study the electronic, structural and transport properties of monoatomic Mo wires encapsulated inside single-walled carbon nanotubes. We used the SIESTA code [1] for the structural relaxation, while the transport properties were calculated with the non-equilibrium Green's functions formalism SMEAGOL [2]. We have simulated Mo wires inside single-walled carbon nanotubes with zigzag and armchair chiralities of different radii. We have found that the ground state of these systems is always formed by non-magnetic Mo dimers (Fig. 1) with interatomic distances similar to those of the periodic monoatomic Mo wire in the free-environment [3]. The minimum radius for a nanotube to be able to encapsulate a monoatomic Mo wire was found to be around 2.8 Å. Equidistant Mo wires, which are magnetic with both an antiferromagnetic and a ferromagnetic spin isomers, are also possible when the Mo concentration is decreased, although they are much higher in energy. We have calculated the band structure, densities of states and transmission channels for different thicknesses and chiralities, and we have then compared with those of the Mo wire in the free-environment and of the empty carbon nanotube (Fig. 2). For certain nanotubes, when we encapsulate a long Mo wire inside it (which is an insulator), the resulting system has a metallic behavior, independently of the insulating or metallic character of the nanotube.

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[3] A. García-Fuente et al., Nanotechnology **21**, 095205 (2010)

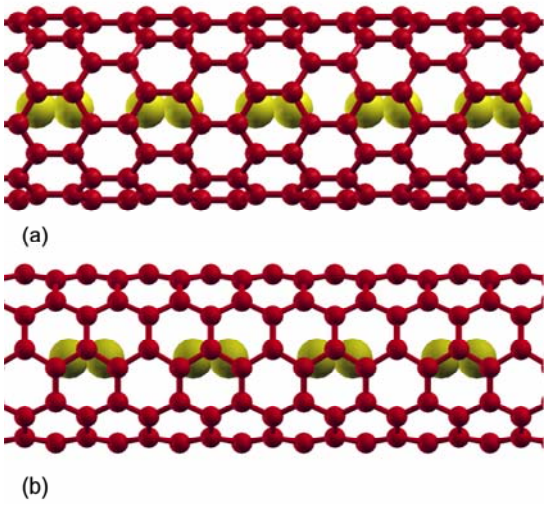

Fig.1: Ground state of a Mo wire inside (a) a (9,0) zigzag nanotube and (b) a (5,5) armchair nanotube.

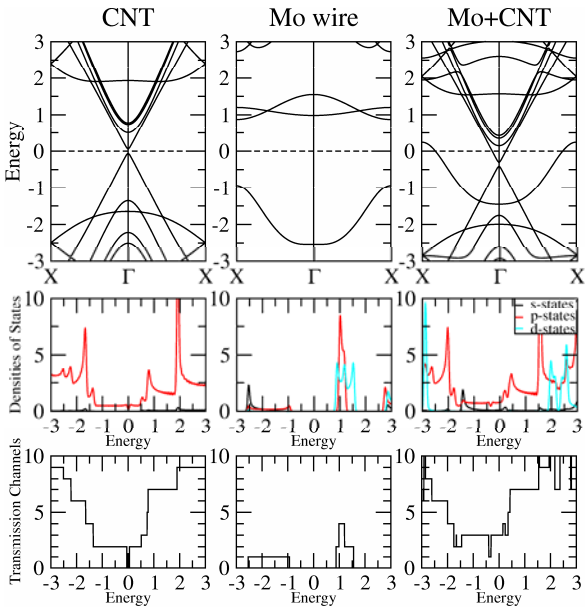

Fig 2: Band structure, projected densities of states and transmission channels of the system formed by a Mo dimerized wire encapsulated inside a (9,0) carbon nanotube compared with those of its components separately. All energies are in eV and referred to the Fermi level.