Impact of dimerization and stretching on the transport properties of molybdenum atomic wires

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We study the electrical and transport properties of monoatomic Mo wires with different structural characteristics. Mo is an interesting metal element as regards its ability to form one-dimensional structures. Recent ab-initio calculations of free-standing Mo atomic clusters have shown that linear atomic chains containing up to four atoms are more stable than two- and three- dimensional structures.[1] On the other hand, individual molybdenum chains have been produced and controlled by encapsulating them inside carbon nanotubes very recently.[2]

Our calculations have been performed within the DFT formalism with the generalized gradient approximation for the exchange and correlation potential. We have used the SMEAGOL code [3] to compute the transmission coefficients and the current using the Landauer formalism:

$$I(V) = \frac{2e}{h} \int dE\ T(E,V)\left(f_L(E,V) - f_R(E,V)\right)$$

As a consequence of Mo having an exact half band filling, the ground state of the Mo wire is formed by tightly bound dimers. We consider first periodic wires with inter-atomic distances ranging between the dimerized wire to that formed by equidistant atoms. The ground state of all the chains is non magnetic. As all these chains are periodic, the transmission coefficients *T(E)* in units of G_0 will just count the number of bands at energy *E*, being $G_0=2e^2/h$ the conductance quantum unit. We find that the dimerized case has a gap in the electronic structure which makes it insulating. As we move to the equidistant case, many occupied and unoccupied bands move gradually towards the Fermi level, and for equidistant chains, as well as for slightly dimerized chains, we have a metallic behaviour (Fig 1).

We also simulate two conducting equidistant one-dimensional Mo electrodes separated by a scattering region which contains a number of dimers between 1 and 6. Even with only 1 dimer, the transmission at the Fermi level falls form 6 to only 1 G_0. As we increase the number of dimers in the scattering region, the transmission at the Fermi level decreases in an exponential way (Fig 2). This means that the transport must be in the tunnelling regime. The I-V characteristics strongly depend on the number of dimers and vary from ohmic to tunnelling, with the presence of different gaps.

The interatomic distances recently measured between Mo atoms in individual monoatomic chains encapsulated inside carbon nanotubes[2] ranged from 3.2 to 3.8 Å. Those wires are then far form being dimerized, but their distances are longer than the distances in the equidistant wire that we have studied. These stretched chains are ferromagnetic, with a full spin polarization, where the magnetic moment is saturated to its maximum possible value of 6 μ_B. This makes the chain an insulator, due to the magnetic splitting that leaves all the majority spin s- and d-states below the Fermi level and all the minority spin s- and d-states above the Fermi level.

References:

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Figures:

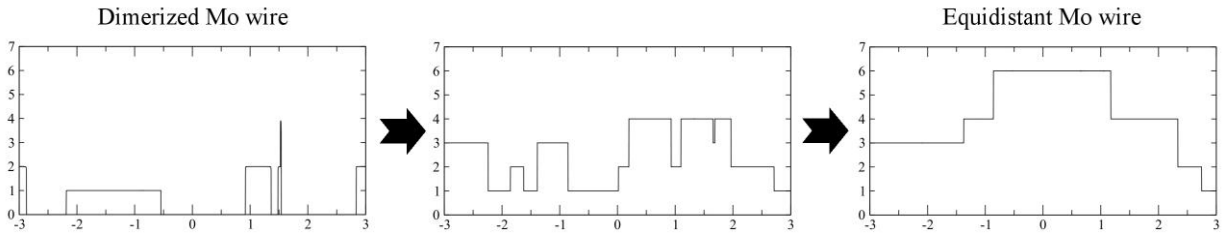

Figure 1: Transmission (G_0) as a function of the energy referred to the Fermi energy (eV) for a Mo atomic wire with the interatomic distance going from the dimerized to the equidistant case.

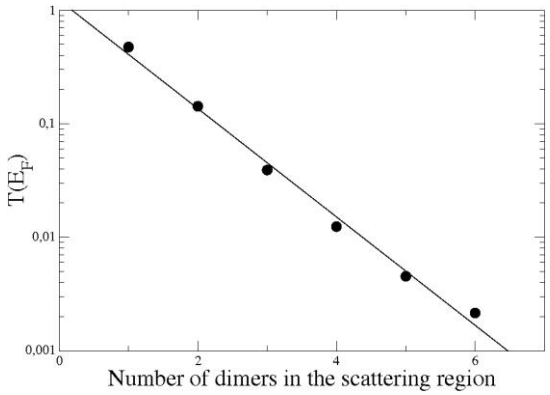

Figure 2: Logarithm of the transmission at the Fermi level as a function of the number of dimers in the scattering region.