THEORETICAL STUDY OF FUNCTIONALIZED NANOTUBES BETWEEN TRANSITION METAL ATOMS

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Functionalized nanotubes [1] are interesting bridging ligands to comunícate paramagnetic transition metals, thus, we can solve the problem of the fast decay of the exchange coupling between this paramagnetic centres at long distance [2]. The mechanism of the exchange interaction is related with a charge transfer processes between the d orbitals of the metal and the π system of the nanotube. Previously, theoretical studies based on density functional theory predicted the presence of strong couplings at very long distances for this kind of systems. This coupling mainly depends of the chirality and nature of the nanotube and the oxidation state of the metal cation; it is stronger through metallic nanotubes than with semiconducting ones in similar length. Now we want to extend this previous work showing results for either metallic or semiconducting chiral nanotubes.

References:

[1] S. Banarjee, M. G. C. Kahn, S. S. Wong, Chem. Eur. J., **9** (2003) 1898.
[2] E. Ruiz, F. Nunzi, S. Alvarez, Nano Letters, **6** (2006) 380.