ENGINEERING THE ELECTRICAL RESPONSE OF NANOWIRES

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Theoretical results for the electronic transport of atomic wires, performed with the code SMEAGOL[1], that combines the Molecular Dynamics Density Functional code SIESTA with non-equilibrium techniques, will be presented.

It will be shown that the conductance oscillations seen in Mechanically Controllable Break Junction experiments of Platinum leads can be explained by the opening and closing of channels as Pt chains are formed in a zigzag arrangement and subsequently stretched to a linear configuration in every pulling cycle.

Results will also be presented for the spin polarized currents that flow through wires of metalic molecules encapsulated inside Single Wall Carbon Nanotubes, where the conductance can be taylored by the appropriate choice of the metallic atom.

[1]Spin and Molecular Electronics in an Atomically Generated Orbital Landscape, A. R. Rocha, V. M. García Suárez, S. W. Bailey, C. J. Lambert, J. Ferrer and S. Sanvito, http://www.smeagol.tcd.ie.