SPIN-DEPENDENT TRANSPORT IN CHAINS OF COBALTOCENES INSIDE CARBON NANOTUBES

V. M. García-Suárez^{1,2}, J. Ferrer² and C. J. Lambert¹

¹Dept. of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom ²Departamento de Física, Universidad de Oviedo, Oviedo 33007, Spain

v.garcia-suarez@lancaster.ac.uk

The encapsulation of molecules inside carbon nanotubes [1] produces new and interesting properties [2,3]. Recently it was demonstrated the possibility of encapsulating cobaltocenes [4], a process which depends strongly on the diameter of the nanotube. Based on this experiment, we have performed a complete series of ab-initio simulations where we studied the energy-dependence on the diameter of the nanotube, the mobility of the molecule inside the nanotube and the magnetic configurations. We also performed transport calculations using the recently developed code SMEAGOL and we found the existence a spin-polarized channel through the molecule which gives a significant ratio of magnetoresistance.

References:

- [1] C. Guerret-Plécourt et al, Nature **372**, 761 (1994).
- [2] Jhinhwan Lee et al, Nature **415**, 1005 (2002).
- [3] T. Mühl et al, Journal of Applied Physics **93**, 7894 (2003).
- [4] R. J. Nicholas (unpublished).