Magnetic Co impurity in Gold Nanowires

EDISON DA SILVA, Instituto de Física “Gleb Wataghin”, UNICAMP, Brazil, RENATO PONTES, ANTONIO J.R. DA SILVA, ADALBERTO FAZZIO, Instituto de Física, USP, Brazil.

Nanoscale electric contacts using suspended gold nanowires (NWs) have recently been made and were imaged by electron microscopy. Using tools derived from Density Functional Theory (DFT) we study the role of magnetic impurities in these NWs with the possibility of spintronic applications. Here we study structural and transport properties of a gold nanowire with one Co impurity as function of tension applied to the NW. Co added new features to the physics of this system. We present studies of structure and also electronic transport using the same DFT formalism [1] that show the effect of the spin anisotropy introduced by Co. In particular, we present results of two geometries, one where the Co atom is connected to two Au atoms of the lead and another where it is in the middle of the suspended neck, in a linear configuration. In the former case we observe an interference between the s and d channels, leading to a Fano-like structure in the transmittance, whereas in the latter configuration due to the local symmetry there is a decoupling between these two channels and the transmittance has a simple peak around the Co d-states, leading to a large spin polarized transport. [1] F. D. Novaes, A.J.R. da Silva, and A. Fazzio, Braz. Jou. Phys. 36 (3A): 799-807 (2006)

Work supported by FAPESP and CNPq. CENAPAD-SP is acknowledged for computer time.

Edison Z. da Silva
Instituto de Física “Gleb Wataghin”, UNICAMP,
CP 6165, 13083-970, Campinas - SP, Brazil

Date submitted: 14 Dec 2007