

Abstract Submitted
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Transport properties of transition metal impurities on gold nanowires¹ RENATO B. PONTES, Physics Institute-USP, EDISON Z. DA SILVA, Physics Institute-UNICAMP, ADALBERTO FAZZIO, ANTÔNIO J. R. DA SILVA, Physics Institute-USP — Performing first principles density functional theory (DFT) we calculated the electronic and transport properties of a Au thin nanowire with transition metal atoms (Mn, Fe, Ni or Co) bridging the two sides of the Au nanowire. We will show that these systems have strong spin dependent transport properties and that the local symmetry can dramatically change them, leading to a significant spin polarized conductance. This spin dependent transport is also associated with the transition metal in the nanowire, in particular with the d-level positioning. Using Co, for example [1], when the symmetry permits the mixing between the wire s-orbitals with the transition metal d-states, there are interference effects that resemble Fano-like resonances with an anisotropy of 0.07 at the Fermi level. On the other hand, if this symmetry decouples such states, we simply have a sum of independent transmission channels and the calculated anisotropy was 0.23. The anisotropies for the other transition metals, as well as calculated transmittances for two Co impurities will also be presented [1] R. B. Pontes, E. Z. da Silva, A. Fazzio and Antônio J. R. da Silva, *J. Am. Chem. Soc.* 130 (30), 9897-903, 2008

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