Abstract Submitted
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Ab initio transport properties of platinum chains calculated by taking into account spin orbit effects VICTOR GARCIA-SUAREZ, Lancaster University, DAVID ZSOLT MANRIQUE, Universidad de Oviedo, COLIN LAMBERT, Lancaster University, JAIME FERRER, Universidad de Oviedo — The transport properties of infinite and finite platinum chains are calculated by using a combination of Density Functional Theory and Non-Equilibrium Green's Functions Formalism, as implemented in the Smeagol Code. We show that spin orbit effects, which are included fully self-consistently in our calculations, are of paramount importance to determine accurately the electronic and transport characteristics of these systems. For infinite chains we find that under special circumstances which depend on the type of chain (linear or zigzag), length and spin orientation relative to the chain, the conductance can be totally suppressed, giving rise to large magnetoresistive ratios. In the case of finite chains between bulk electrodes the spin-orbit effect plays also a crucial role and gives results which agree better with experiments.

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