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Manganese Phthalocyanines on manganese surfaces: An ab-initio approach to the tunneling magnetoresistance MARIA SORIANO, JUAN JOSE PALACIOS, Universidad Autonoma de Madrid — We have performed computational studies of spin polarized transport based on Density Functional Theory (DFT) using a non-equilibrium Green's functions formalism implemented in our ANT code [1] to compute tunneling magnetoresistance (TMR) on different manganese based systems. Specifically we present results for STM tips on a clean manganese surface, which is well known to show an antiferromagnetic coupling between layers when grown on an iron surface. In this system we have studied the dependence of the TMR on the tip-surface distance, the position of the tip, and on the bias voltage. Also we present a comparison between the Landauer formalism and the Tersoff-Hamman approach, usually used in this context. Finally we analyse the interaction between Manganese Phthalocyanine (MnPc) molecules on the manganese surface, focusing on the TMR signature and its dependence on the different adsorption sites.

[1] J.J. Palacios et. al. Ab-initio Quantum Transport (ANT). alacant.dfa.ua.es

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