EMERGENCE OF HALF-METALLICITY IN NANOSCALE NIO: NIO CHAINS AND OXIDIZED NI NANOCONTACTS

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Whether or not ferromagnetic (FM) nanocontacts display large magnetoresistance (MR) is still a matter of debate [1-3]. From the theory side it has been shown [4] that MR in *pure* Ni nanocontacts is certainly not large in good agreement with recent experiments [5]. Here we explore the effect of oxygen atoms on the electronic structure and transport of nickel nanocontacts.

While bulk NiO is an antiferromagnetic (AF) charge-transfer insulator [6] the situation changes completely at the nanoscale: In a perfect one-dimensional NiO chain the electron transfer from Ni to O is less favourable than in the bulk due to the lower coordination of the atoms and the corresponding decrease in Madelung binding energy. Thus the O 2p shell is only partially filled and can form a spin-polarized conduction band by hybridization with Ni 3d orbitals. Indeed our ab-initio calculations show that a perfect one-dimensional NiO chain becomes a *half-metallic* conductor with ferromagnetic (FM) order when stretched out of equilibrium whose conduction bands are composed of 2p and 3d minority-spin orbitals.

Furthermore ab-initio quantum transport calculations of a Ni nanocontact with a single oxygen-atom adsorbed between the tip atoms (see inset of Fig. 1) show that the half-metallicity of the perfect FM NiO chain translates into strongly spin-polarized electron transport there for the case of parallel alignment of the electrode magnetizations (left panel of Fig. 1). An orbital eigenchannel analysis [7] reveals that two open transport channels contribute to the overall conductance. The transport channels are composed of spin-polarized O 2p-orbitals hybridized with 3d-orbitals of the Ni tip atoms in perfect analogy to the case of the one-dimensional chain. For antiparallel alignment of the electrode magnetizations the conduction is strongly suppressed (right panel of Fig. 1) resulting in very large MR ~ 90%. Thus the presence of oxygen-adsorbates in the contact region could possibly explain the very high MR values obtained by some groups.

References:

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Figures:

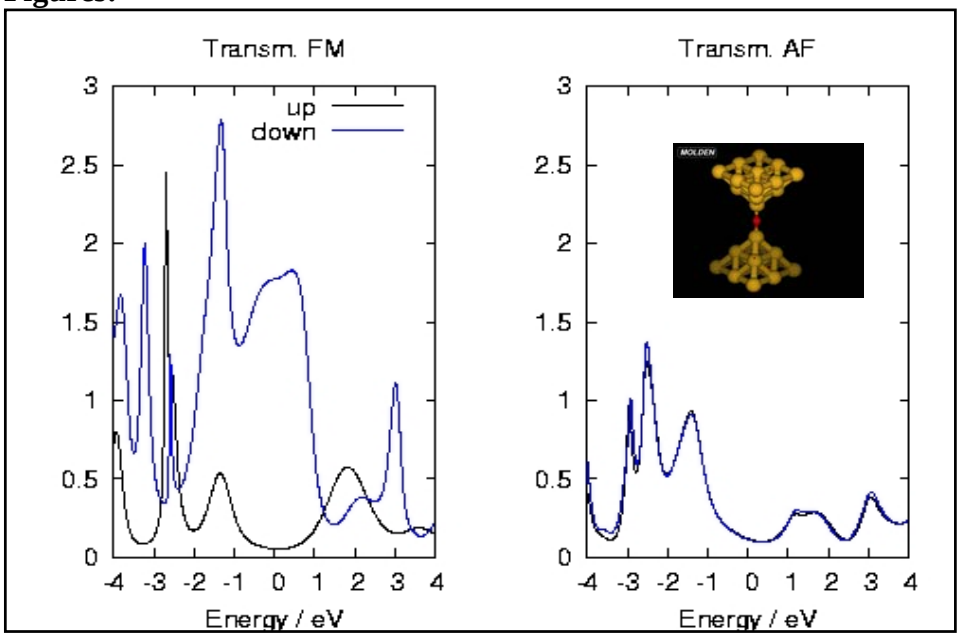

Fig. 1 Transmission function through a single oxygen atom in a Ni nanocontact for FM order (left) and AF order (right) of Ni atoms in the two electrodes. The inset in the right panel shows the geometry of the contact with the adsorbed O atom for which the transmission functions were calculated.