Spin-dependent all-electron tunneling through junctions

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In recent years one is witnessing an increasing experimental effort in preparing junctions made of ferromagnetic leads and a variety of different barrier materials including simple oxides, semiconductors, piezoelectrics, ferroelectrics and multiferroics. The most prominent one is certainly the tunneling magneto-resistant (TMR)-system Fe/MgO/Fe [1], which is the core of a non-volatile memory cell of a magnetic random access memory. Characteristic to all systems is that structural and chemical details at the interface determine substantially the tunneling characteristics, which makes the description of the transport properties a challenging task.

In order to provide an understanding of the transport properties of these systems from an *ab initio* description of the electronic structure, giving account of the complex interplay between the electronic structure, the details of the atomic arrangement and the magnetism in these planar junctions we developed an electronic transport code in the context of an all-electron full-potential scheme. We implemented the Green-function embedding formalism within the framework of the full-potential linearized augmented plane wave (FLAPW) method [2] as implemented in the `FLEUR`-code [3]. This approach allows the calculation of the embedded Green function of the finite scattering region with the correct boundary conditions of attached semi-infinite leads, which appear as additional energy-dependent non-local potentials in the transport calculations.

We focus on results of the Fe/MgO/Fe based system [4, 5], for which we show that very small changes at the interface can have drastic effects on the conductance. If time permits we will present a second system: a $SrRuO_3/SrTiO_3/SrRuO_3$ three-layer junction, where $SrRuO_3$ is a ferromagnetic metal and $SrTiO_3$ forms an insulating barrier. We discuss the role of the interface structure and chemistry on the spin-polarization of the electronic transmission in these systems.

References

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