Multiferroic interfaces of mixed valency systems studied from first principles

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The phenomenon of multiferroicity, which allows, in particular, coexistence of magnetic and ferroelectric ordering in one material [1,2], offers many interesting applications in spintronics. Rich physics is observed when the two order parameters are cross-coupled, giving thereby the possibility to control the magnetization by applying an external electric field and vice versa. This allows more versatile control of electron transport in multiferroic devices, as demonstrated by recent experiments on oxide-based tunnel junctions [3-5] where the possibility to change the magnitude [3] and even the sign [4,5] of the TMR effect by means of the ferroelectric switching in the tunneling barrier was confirmed.

In this talk, the interplay between multiferroicity and tunneling electron transport will be demonstrated for the recently measured LSMO/PZT/Co tunnel junctions [4,5] where the inverse TMR effect can be induced for a certain polarization state of the PZT barrier. First-principle study of the underlying electronic phenomena was performed in this work using density functional theory in conjunction with the Landauer-Buettiker formalism for the tunneling transport. As a result, the key factors for the tunneling behavior were determined.

Although pronounced magnetoelectric coupling effect is predicted for both interfaces in the LSMO/PZT/Co junction [6], it is not solely responsible for the TMR sign change observed in experiment. Crucial factor is the spin polarization of both electrodes (LSMO and Co) as well as the wavefunction symmetry at the Fermi energy. Another issue of interest is the effective barrier thickness for tunneling electrons [5,6]. Its variation under the polarization reversal is determined mostly by the assymetric interface terminations and a local metallization of PZT due to the charge transfer from the ferromagnetic electrodes.

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