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Electron tunneling in epitaxial magnetic tunnel junctions[1]

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The remarkable progress in the performance of tunneling magnetoresistance (TMR) junctions using MgO as the barrier layer, has confirmed the theoretical prediction of a very high TMR ratio from first-principles calculations [1,2]. The theoretical prediction was based on the understanding of the band filtering effect by a class of barrier materials, including ZnSe, and even vacuum, in addition to MgO, along particular crystalline orientations. The combination of the preferential filtering for the electrons with the Δ_1 symmetry by the barrier layer, and the presence of the Δ_1 band only in the majority spin channel of Fe, FeCo and Co electrodes, results in the high TMR ratio previously believed only achievable with half-metallic electrodes. Here we show that the remarkable agreement between the experiment and the first-principles theory goes beyond the TMR. The effects of barrier thickness, interface resonance states, and quantum confinement calculated from the first-principles for MgO based magnetic tunnel junctions are compared with experimental data. In addition to excellent agreement for each case, additional insights are obtained from the first-principles calculations that are otherwise not directly available from the experiments. We also discuss other candidate materials for high TMR junctions.

[1] W. H. Butler, X.-G. Zhang, T. C. Schulthess et al., Phys. Rev. B 63, 054416 (2001).
[2] J. Mathon and A. Umerski, Phys. Rev. B 63, 220403 (2001).

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