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First-principles prediction of high Curie temperature for ferromagnetic bcc-Co and its relation to Co/MgO/Co magnetic tunnel junctions MARJANA LEZAIC, IFF, Research Center Juelich, PHIVOS MAVROPOULOS, STEFAN BLUGEL — We determine from first principles the Curie temperature of bulk Co in the ground state hcp phase and the metastable fcc and bcc phases. For fcc-Co we found a Curie temperature of T_{C}(fcc-Co) = 1280 K, in reasonable agreement with experimental results. For bcc-Co, a Curie temperature of T_{C}(bcc-Co) = 1400 K is predicted. This suggests that bcc-Co/MgO/bcc-Co tunnel junctions offer high tunneling magnetoresistance ratios even at elevated temperatures, giving them an advantage over Fe/MgO/Fe junctions. T_{C}(bcc-Co) appears robust under tetragonalization upon epitaxial growth on MgO, in contrast to Fe for which T_{C}(bcc-Fe) is found to drop by more than 20% (from 970 K to 750 K) upon such a tetragonalization. We find that FeCo alloys have an even higher T_{C}, as high as 1660 K for ordered FeCo. We discuss the origin of these effects in terms of the electronic structure and densities of states. The Curie temperatures are calculated by mapping *ab initio* results to a Heisenberg model, which is solved by a Monte Carlo method.

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