Role of heavy transition metals on magnetic anisotropy in TM/Fe/MgO(001)

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Capping by 5*d* transition metal (TM= Hf, Ta, W, Re, Os, Ir, Pt, and Au) on a typical magnetic tunnel junction Fe/MgO(001) is investigated using a first-principles calculations for their magnetism and magnetocrystalline anisotropy (MCA), which exhibits systematic changes with the atomic number of the capping TM. The early (late) TMs, less (more) than half-filled, show antiparallel (parallel) magnetizations with respect to Fe. This magnetic behavior is explained by kinetic exchange energy gain of electrons in the minority spin states of TMs and Fe. The cappings of the center TMs, Re, Os, and Ir, enhance MCA of Fe/MgO(001) significantly, particularly in Os/Fe/MgO(001) perpendicular MCA (PMCA) reaches gigantic 8.52 meV/cell. On the other hand, the cappings by the very early and the late TMs, Hf, Ta, and Au, do not change much the MCA of of Fe/MgO(001), while the capping by W and Pt turn PMCA to in-plane. The variation of MCA is due to the shifting-down of the TM *d*-bands as the number of valence electrons increase.

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