Giant Perpendicular Magnetic Anisotropy of a Fe(001) Surface: A Density Functional Study

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ABSTRACT

We predict agigantic perpendicular magnetocrystalline anisotropy (MCA) in Fe (001) capped by *5d* transition metal (TM) overlayers by using first principles calculations. Analysis of atom-by-atom contribution to MCA reveals that gigantic MCA as large as 11 meV/TM originates not from Fe atoms but from the *5d* TMs through the strong spin-orbit coupling. More specifically, it is the hybridization between TM and Fe d orbitals that also induces non-negligible magnetic moments in TM. Furthermore, spin-channel decompositions of MCA matrix with and without the presence of Fe substrate identify the electronic origin of the perpendicular MCA that the down-down channel contribution plays the most crucial role for the sign changes of MCA of TM overlayers upon the hybridization with Fe-*3d*.

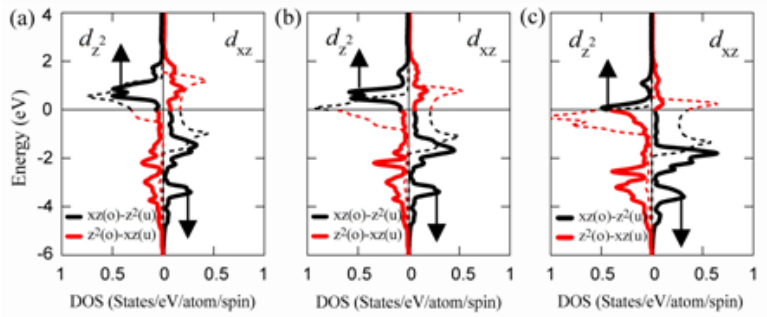

FIG. 1.The d_z^2(the left side)- and $d_{xz/yz}$(the right side)-projected minority spin DOS of (a) Os, (b) Ir, and (c) Ptatom of the free-standing TM ML's (thin dashed lines) and of TM/Fe(001) (thick solid lines).