

# Materials with large MCA and design principles of large MCA

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We review here recent studies on MCA, more specifically, Fe/MgO, FeRh films, and Fe layer with transition metal capping using first-principles calculations. While d-d hybridization between Fe and transition metals enlarges spin-orbit matrix, the large MCA found in Fe/MgO can be attributed to perfect epitaxy of the interface rather than widely accepted hybridization between Fe and O. Furthermore, design principles of MCA will be presented relying on the irreducible representation of crystal symmetry. Some other spin-orbit related phenomena, Dzyaloshinskii-Moriya interaction, are discussed briefly within scheme of density functional theory.