A first principles study of electric field effect on magnetization and magnetocrystalline anisotropy: FeCo and FeCo/MgO

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The magnetic and electronic properties of bulk and thin films of FeCo and FeCo/MgO have been investigated using first-principles calculations. For the thin film FeCo, as number of layers increases from a monolayer (ML) to 5 MLs, surface magnetic moments of Fe are feasibly decreased from 3.19μ_B to 2.97μ_B, whereas it is enhanced from 2.16 to 2.71 for Co case. Those magnetic moments at surface are much larger than that in bulk FeCo. However, in the presence of the substrate MgO, magnetic moments of interface Fe and Co are dramatically decreased caused by interaction with the MgO substrate. Additionally, the magnetocrystalline anisotropy (MCA) energies of FeCo/MgO film enhanced to +1.74 meV/cell in the 2ML, but it showed in-plane MCA in the 3ML to 5ML FeCo/MgO.

Furthermore, by applying electric field along z axis, magnetic moment of Fe atom in Fe/MgO is increased from 2.82μ_B (EF=0 eV/Å) to 2.87μ_B (EF=1 eV/Å). Additionally, MCA at the interface can be modified by an applied electric field. We will discuss in detail in the presentation the external electric field effect on MCA depending on thickness of FeCo films on MgO substrate.