**First-Principles Density Functional Study in the Magnetically and Electrically polarized Pt/CoO/ZnO**

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Non-volatile and low-energy-consumption memory, for examples, Magnetoresistive Random Access Memory (MRAM) or Ferroelectric RAM (FeRAM), has been investigated for over ten years. Recently the junction of CoPt/MgZnO was fabricated and investigated as an interesting hybrid [1]. Atomic layer stacking of CoPt has a large magnetic anisotropy energy (MAE) because of large spin-orbit interaction (SOI), and wurtzite-ZnO can provide a spontenious electric polarization depending on its surface edge. The CoPt magnetic metal with ZnO-based tunnel junction is a candidate of materials for the new device hybridizing MRAM and FeRAM. The electronic structure at the ferromagnetic/ferroelectric interface is so mysterious that the mechanism of interaction between ferromagnetics and ferroelectrics has still been veiled.

We investigated electronic structure of Pt(111)/CoO/ZnO(0001) slab system by using a first-principles calculation based on density functional theory. The method covers the effects of magnetic and electric polarizations for slabs [2,3]. To analyse modulation with respect to the electric polarization direction of ZnO, we considered that two ZnO structures; Zn adjacent to CoO plane as P+, and O adjacent to CoO as P-. The in-plane lattice constant was fixed a ZnO value extracted from the bulk and we induced out-of-plane structural relaxation for P+ and P-, respectivly. After a self-consistent computation, we confirmed both a spin polarization in PtCo layer and a spontenious electric polarization of ZnO, simultaneously. The direction of P+ is toward CoO, and the direction of P- is opposite. In each resulting slab, the electric polarization of ZnO is cancelled out by the electrostatic potential to fulfill a Poisson’s equation. The result shows that in P+ electrons around CoO tend to sweep out to ZnO side (electron depletion state). On the other hand, electrons in P- is attracted to CoO side (electron accumulation state). This is consistent with the number of electrons in Co atomic sphere. We also analysed partial density of states (PDOS). There are large exchange splittings in the PDOSs of Co and adjacent Pt. There is a large component in d-orbital of Co and d(3z2-r2)-orbital of Pt around the Fermi energy. These states have large difference between P+ and P-.In particular, the peak of d(3z2-r2)-orbital in Pt gets down across the Fermi energy from P+ to P-. These changes in electronic structure might contribute to a favor of in-plane easy axis because of a large SOI of Pt. In the presentation, we will discuss electronic structures like a multi-ferroic material in terms of ferromagnetic and ferroelectric properties in the interface.

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