Analysis of the magnetic structure and spin exchange interactions of multiferroic YBaCuFeO$_5$ by first principles DFT calculations

JERRY BETTIS, YUEMEI ZHANG, C. LEE, MIKE WHANGBO — In the layered perovskites RBaCuFeO$_5$ (R = Y, Lu, Tm), the CuFeO$_9$ dumbbells made up of apex-sharing CuO$_5$ and FeO$_5$ square pyramids share their basal corners to form perovskite layers, and the resulting CuFeO$_5$ slabs are stacked along the c-direction. Recently, these compounds were found to exhibit ferroelectric polarization when a modulated magnetic component is superposed on their antiferromagnetic structure. To help understand this finding, we examined the spin exchange interactions between the Fe$^{3+}$ ($d^5$) ions, between the Cu$^{2+}$ ($d^9$) ions, and between the Fe$^{3+}$ and Cu$^{2+}$ ions on the basis of DFT+U and DFT+U+SOC calculations for YBaCuFeO$_5$. The ferroelectric polarization of YBaCuFeO$_5$ was also calculated for several modulated magnetic structures that were constructed based on the cone-model.

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