

Abstract Submitted
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Analysis of the magnetic structure and spin exchange interactions of multiferroic YBaCuFeO₅ by first principles DFT calculations JERRY BETTIS, YUEMEI ZHANG, C. LEE, MIKE WHANGBO — In the layered perovskites RBaCuFeO₅ (R = Y, Lu, Tm), the CuFeO₉ dumbbells made up of apex-sharing CuO₅ and FeO₅ square pyramids share their basal corners to form perovskite layers, and the resulting CuFeO₅ 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 Fe³⁺ (d⁵) ions, between the Cu²⁺ (d⁹) ions, and between the Fe³⁺ and Cu²⁺ ions on the basis of DFT+U and DFT+U+SOC calculations for YBaCuFeO₅. The ferroelectric polarization of YBaCuFeO₅ was also calculated for several modulated magnetic structures that were constructed based on the cone-model.

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