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Magnetic structure of hexagonal YMnO3 compound: A non-collinear spin DFT study

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The hexagonal $YMnO_3$ (h-YMO) is one of the most studied magnetoelectric materials because of its suitability for usage in ferroelectric (FE) memories and due to the intriguing coexistence of ferroelectricity and magnetism. It has a high ferroelectric-paraelectric transition temperature (T_c ~ 1258 K), and a low antiferromagnetic (AFM) – paramagnetic (PM) transition temperature (T_n ~ 75 K). For $T < T_n$ the h-YMO is simultaneously AFM and FE, exhibiting a clear magnetoeletric characteristic. The magnetism in this compound arises from Mn^{3+} ions, in $3d^4$ configuration, with high spin state, S = 2. Despite numerous investigation about of the h-YMO magnetic structure, it is still under debate in the literature [1-3]. In this work we performed a non-collinear spin density functional theory (DFT) study in order to obtain the magnetic ground state of the h-YMO compound. The calculations were carried out using a full potential linearized augmented plane wave method as embodied in the Elk computer code. With this computational tool, we could simulate all magnetic configurations described by the experiments for the h-YMO crystal with and without SOC interaction. The lowest energy was found to $P6'_3$ magnetic structure when the SOC are present. Our results shown that the inclusions of the SOC interaction, in fact, give rise a small FM component along the c axis in agreement with previous experimental observation [3].
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