Spin-orbit Coupling Effects in Multiferroic Bi_2FeCrO_6

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For application in integrated sensors or devices, functional materials are used in the form of thin films. Ferroelectricity and many other properties of multiferroic materials, such as the magnetocrystalline anisotropy, are strongly related to the material crystal structure. Because fundamental physics of multiferroic materials is rich, theoretical studies are of great importance, since it is extremely difficult to understand the intrinsic material properties using only experimental data. An example of multiferroic material having the potential to revolutionize electronic industry is the rhombohedral double-perovskite Bi_2FeCrO_6 (BFCO) owing to its good ferroelectric and magnetic properties at room temperature that were both theoretically predicted by ab-initio calculations [1] and experimentally demonstrated on epitaxial thin films [2]. To complement these studies, theoretical investigations have been performed in order to analyze the spin-orbit coupling (SOC) effects on the magnetic and ferroelectric properties of BFCO. Using first-principles density functional theory (DFT) calculations within the VASP package, investigations were performed for both collinear and non-collinear spin structures of BFCO, respectively. Exchange and correlation effects were treated using the local density approximation plus Hubbard potential, on the different possible high spin (HS) and low spin (LS) states of the ferromagnetic (FM) and ferrimagnetic (FiM) spin arrangements.

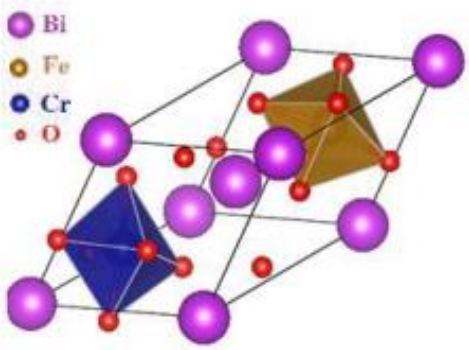

Figure 1 Structure of the BFCO.

In the case of collinear spin calculations without SOC, the existence of four competing phases (FMHS, FMLS, FiMHS and FiMLS) with distinct electronic and magnetic properties was found, in agreement with recent published theoretical results [3]. The FiMHS state was found to be the

most stable, with a total magnetic moment $|M_{BFCO}|$~$2\mu_B$/cell, and a computed spontaneous polarization of P_s=79.1 [$\mu C/cm^2$] in agreement with reported data [1]. When SOC was considered, the calculations also showed the existence of the above four stable states, FiMHS remaining the most stable state. It was found that magnetization is somewhat higher, namely $|M_{BFCO}|$=2.005 μ_B/cell, when the total magnetization vector is parallel to the direction (1 1 -2). It was also shown that, the obtained magnetizations does not have a preferred direction in the HS states, but show deviation from the direction (1 1 1) in the LS states, due to structural distortions, with energy minimized in the direction ~(2 1 1). Spontaneous polarizations computed for optimized structures using the Berry-phase method, were found to be slightly higher when SOC is considered, namely P_s~81.5 [$\mu C/cm^2$] for FiMHS.

Additionally, comparing the Fe-O and Cr-O bond lengths in the FeO_6 and CrO_6 octahedra, it was found that the Cr-O bonds and Cr^{3+} magnetic moments have non-significant changes (smaller than 0.7% of the bond length) when SOC is considered, while Fe-O bonds and Fe^{3+} magnetic moments exhibit substantial changes (up to 6.9% of the bond length).

References

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