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Evolution of weak ferromagnetism in $BiFeO_3$ under applied epitaxial strain[1] HEMANT DIXIT, JUN HEE LEE, VALENTINO R. COOPER, Oak Ridge National Lab — The magnetoelectric effect has been a focus of research in multiferroic materials due to potential applications in magnetic data storage, spintronics and memory devices. We perform first principles calculations based on density functional theory to explore the evolution of weak ferromagnetism under compressive and tensile strains in $BiFeO_3$. An isosymmetric phase transition between the rombohedral ground state and strained phases (Cc space group) is considered which confines the polarization vector to rotate in the (110) plane. For the ground state, we find that the easy spin axis is degenerate in a plane perpendicular to the polarization direction. This weak ferromagnetic moment also persists for the tested strain values (up to $\pm 5\%$). Under compressive strains, the easy spin axis is also degenerate in a plane perpendicular to the polarization vector. On the other hand for tensile strain the weak ferromagnetic ordering is stabilized along the [1-10] direction. Further, calculated Dzyaloshinskii-Moria interactions help us to understand the stabilization of weak ferromagnetic moments in the tensile region. Our study thus offers useful insights for manipulating the magnetic response and utilizing the magnetoelectric effect.

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