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Strain control of magnetization in $TbFe_2$ RITIKA DUSAD, School of Applied and Engineering Physics, Cornell University, M.D. JOHANNES, Naval Research Laboratory, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — Magnetostrictive materials change their shape upon application of strain and can be used as actuators and sensors. In this work, we perform a computational analysis of a highly magnetostrictive compound, $TbFe_2$, to understand how the lattice and magnetization couple. We use Density Functional Theory (DFT) to investigate the magnitude and direction of the metallic moment as a function of pressure. The localized nature of Tb f-electrons classify this compound as "strongly-correlated" and necessitate the simultaneous use of spin-orbit coupling to treat magnetostriction and the DFT+U methodology to capture the physics of the f-electrons. Although, the energy scales involved in spin-lattice interactions are extremely small, we were able to correctly reproduce the correct magnetic ground state and the experimentally observed ferrimagnetic coupling between Tb and Fe atoms in $TbFe_2$. The easy axis in $TbFe_2$ points along one of its body diagonals, which makes the shape of the crystal rhombohedral. Switching of magnetization between the easy axes requires the magnetization to pass through one of the [100] directions. In our study we show that by applying isotropic strain on $TbFe_2$ crystal, we can decrease the energy barrier between [111] and [100] magnetization directions of the crystal.

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