

Abstract Submitted  
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**Tuning the magnetic ordering in  $\text{EuTiO}_3$  through doping** ZHIGANG GUI, ANDERSON JANOTTI, Univ of Delaware —  $\text{EuTiO}_3$  (ETO) is a complex oxide that displays strong spin-lattice coupling, large magnetoelectric effects, and undergoes a series of structural and magnetic phase transitions when subjected to pressure or epitaxial strain. ETO adopts a cubic structure and is paramagnetic at high temperatures, while at very low temperatures it transforms to an antiferrodistortive tetragonal structure with a G-type antiferromagnetic (AFM) ordering. Several approaches have been presented to tune the magnetic ordering from the G-type antiferromagnetism to the F-type ferromagnetism, often relying on external pressure or epitaxial strain. Doping through substitution of trivalent species on the europium sites or creation of oxygen vacancies have also been proposed to lead to ferromagnetism. However, the fundamental mechanism by which excess electrons from impurities or defects lead to ferromagnetic ordering is unclear. In this study, we explore the effects of doping on the magnetic ordering in  $\text{EuTiO}_3$  through first-principles calculations. We show how itinerant carriers in the Ti- $d$ -derived conduction-band states interact with europium  $f$  states, inducing an alignment of the large moments on the europium ions. The effects of doping of different types of magnetic ordering are considered, a

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