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Electronic structure of $EuTiO_3$ and related heterostructures ANDERSON JANOTTI, ZHIGANG GUI, University of Delaware — $EuTiO_3$ (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. 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 ferromagnetism, often relying on external pressure or epitaxial strain. Doping through substitution of trivalent species on the europium site 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 $EuTiO_3$ through first-principles calculations. In special, we discuss how ferromagnetic ordering can be stabilized by means of charge transfer across the interface in polar/nonpolar complex-oxide heterostructures.

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