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Itinerant ferromagnetism in the oxygen-deficient EuTiO₃: A first-principles investigation¹ HAI-XIA CAO, HAI-SHUANG LU, TIAN-YI CAI, SHENG JU, Department of Physics, Soochow University — Effects of oxygen vacancy on the electronic structure and magnetism in the quantum paraelectric $EuTiO_3$ were investigated from first-principles. In contrast to antiferromagnetism in the pristine $EuTiO_3$, itinerant ferromagnetism was revealed in the oxygen-deficient $EuTiO_3$. The origin lies in the spin-polarized Ti 3d states, which mediate a ferromagnetic exchange interaction between almost localized Eu 4f spins. In addition, this ferromagnetic exchange coupling was strengthened via the partial occupation of Eu 5d states. These findings not only explain the observation of ferromagnetism in the unstrained $EuTiO_3$ thin films, but also demonstrate the potential application of $EuTiO_3$ in magnetoelectronics.

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