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Electron Correlation in Oxygen Vacancy in $SrTiO_3$[1] CHUNGWEI LIN, ALEXANDER A. DEMKOV, Department of Physics, University of Texas at Austin — Oxygen vacancies are an important type of defect in transition metal oxides. In $SrTiO_3$ they are believed to be the main donors in an otherwise intrinsic crystal. At the same time, a relatively deep gap state associated with the vacancy is widely reported. To explain this inconsistency we investigate the effect of electron correlation in an oxygen vacancy (OV) in $SrTiO_3$. When taking correlation into account, we find that the OV-induced localized level can at most trap one electron, while the second electron occupies the conduction band. Our results offer a natural explanation of how the OV in $SrTiO_3$ can produce a deep in-gap level (about 1 eV below the conduction band bottom) in photoemission, and at the same time be an electron donor. Our analysis implies an OV in $SrTiO_3$ should be fundamentally regarded as a magnetic impurity, whose deep level is always partially occupied due to the strong Coulomb repulsion. An OV-based Anderson impurity model is derived, and its implications are discussed.

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