

Abstract Submission Template

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Plentiful magnetic moments in oxygen deficient SrTiO₃

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-abstract-

Correlated band theory calculations based on the DFT+U approach are employed to investigate oxygen-deficient SrTiO₃. We show that the appearance of magnetism in oxygen vacancies is not determined solely by the presence of a single oxygen vacancy, but by the density of free carriers and the relative proximity of the vacant sites. While an isolated vacancy behaves as a non-magnetic double donor, manipulation of the doping conditions allows the stability of a single donor state with emergent local moments. For clusters of vacancies, different kinds of Ti atomic orbital hybridization are described as a function of the doping level and defect geometry. Our description of the charged clusters widens the previous descriptions of mono and multi-vacancies and points out the importance of the controlled formation of defects for the realization of transition metal oxide based devices with a desirable magnetic performance.

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