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Magnetism and metal-insulator transition in oxygen deficient SrTiO3[1] ALEJANDRO LOPEZ-BEZANILLA, Argonne Natl Lab, P. GANESH, Oak Ridge National Lab, PETER LITTLEWOOD, Argonne Natl Lab — We report new findings in the electronic structure and magnetism of oxygen vacancies in SrTiO3. By means of first-principles calculations we show that the appearance of magnetism in oxygen-deficient SrTiO3 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. Strong local lattice distortions enhance the binding of this state. Consequently we find that the free-carrier density and strain are fundamental components to obtaining trapped spin-polarized electrons in oxygen-deficient SrTiO3, which may have important implications in the design of switchable magneto-optic devices.

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