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Oxygen vacancy driven structural and orbital reconstruction on $SrTiO_3$ surface and subsurface CHANDRIMA MITRA, CHUNGWEI LIN, ALEXANDER A. DEMKOV, University of Texas at Austin — The role played by oxygen vacancies in bringing about important structural and electronic changes on oxide surfaces and interfaces have been a subject of intense scientific study. From two-dimensional electronic conductivity to the formation of magnetic states, oxygen vacancies have been suggested to be responsible for introducing a variety of interesting physical effects in bulk oxides and their surfaces. In this work, we employ Density Functional theory to perform first principles calculations of oxygen vacancy defects on $SrTiO_3$ surface and subsurface. In a defect free $SrTiO_3$ surface, the surface Ti atoms have conduction bands whose lower end comprises of split t_{2g} states (lower lying degenerate d_{xz} and d_{yz} states and the upper lying d_{xy} state). The upper conduction bands consist of split e_g states where the d_z^2 orbital is shifted lower in energy with respect to the $d_{x^2-y^2}$ orbital. In the presence of an oxygen vacancy, orbitals reorder and the Ti d_z^2 orbitals, (which also hybridizes itself with Ti $4s$ state and the neighboring oxygen p states) gets pushed down and occupied leading to the formation of a defect state. Formation energies of oxygen vacancies on the surface and subsurface of $SrTiO_3$ will be presented and the possibility of vacancy induced magnetic states on $SrTiO_3$ surface will be discussed.

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