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Nature of localized states induced by an oxygen vacancy in $SrTiO_3$[1] CHUNGWEI LIN, CHANDRIMA MITRA, ALEXANDER DEMKOV, Department of Physics, University of Texas at Austin — Combining the density function theory and model analysis, we study the nature of localized states induced by an oxygen vacancy (OV) in $SrTiO_3$. The key effect caused by an OV is that it introduces a local mixing between $3z^2 - r^2$ and $4s$, $4p$ orbitals of Ti next to the vacancy. According to our analysis, the OV-induced localized state is highly one-dimensional and is mainly composed of Ti $3z^2 - r^2$ orbitals along the Ti-OV-Ti axis (defined as the z-axis) and Ti $4s$, $4p$ at the OV site. Ti t_{2g} based localized states are ruled out. We suggest the $4s$, $4p$ components of the OV induced localized state should be reflected in the x-ray adsorption spectroscopy when Ti $4s$, $4p$ are served as final states. Our analysis and conclusion apply to general transition metal perovskites.

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Chungwei Lin
Department of Physics, University of Texas at Austin

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