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Oxygen vacancy induced localized state in rutile TiO_2 ¹ DONGHAN SHIN, CHUNGWEI LIN, ALEXANDER A. DEMKOV, Univ of Texas, Austin — Titanium dioxide (TiO_2) is as a promising material for several applications including photocatalysis, solar cells, spintronics and memory devices. Oxygen vacancies (OV) act as active sites for water dissociation and induce ferromagnetism in the bulk. Using density functional theory (DFT) and model Hamiltonian analysis, we investigate the localized states induced by an OV in rutile TiO_2 . We identify two classes of localized states: a hybrid and polaron states. The hybrid state is caused by the orbital overlap between three Ti atoms next to a vacancy and is mainly derived from the Ti e_g orbitals. The polaron state is caused by the local lattice distortion and is mainly composed of one particular t_{2g} orbital from a single Ti atom. The first principles calculation shows that the polaron state is energetically favored, and the tight-binding analysis reveals the underlying connection between the bulk band structure and the orbital character of the polaron. Their respective spin moments are deduced from the on-site electron correlation.

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