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Interface orientation dependent carrier distribution in $LaAlO_3/SrTiO_3$ heterostructures TULA R. PAUDEL, EVGENY Y. TSYMBAL, Department of Physics and Astronomy & Nebraska Center for Materials and Nanoscience, University of Nebraska, Lincoln, NE 68588 — Carrier distribution in widely studied $LaAlO_3/SrTiO_3$ heterostructures depends upon the directionality of the interface. From the first-principles calculations, we find that, for the (001) interface, most carriers are localized at the interface and have the d_{xy} character, which decays away from the interface on the scale of 1 nm. The d_{yz}andd_{zx} carrier concentration increases, peaks at about three unit cells (1.15 nm), and then decays very slowly away from the interface. For the (111) interface, we find that the total carrier distribution is similar to that of d_{yz} and d_{zx} in the (001) heterostructure. It has a maximum that lies at about four-bilayers (0.89 nm) away from interface and then decays very slowly producing a long-ranged tail. This difference in the carrier distribution is controlled by the d-orbital splitting which depends on the interface orientation. For the (001) interface, the tetragonal distortion brings the in-plane d_{xy} orbital to about 0.5eV below the Fermi energy, creating a deep localized state, whereas the d_{yz} and d_{zx} orbitals are much shallower and thence less localized. For the (111) interface, the rhombohedral distortion splits the $d-$orbitals by about 0.1 eV so that they are all located in vicinity of the Fermi energy and therefore less localized at the interface.

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