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Electron Accumulation in LaAlO3/SrTiO3 Interfaces by the Broken Symmetry of Crystal Field

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Using ab initio calculations, we reveal the origins of the extraordinarily increased electric conductivity of the LaAlO3/SrTiO3 interface. In both of the two (LaAlO3)m/ SrTiO3 heterojunction models (m=3, 5), the oxygen atoms in the cells were displaced toward the n-type interface and the Ti-centered octahedron structure was compressed along the [001] direction by the atomic reconstructions at the (LaAlO3)m/(SrTiO3)4 interfaces. As a result, the 3dxy orbital of the Ti atom was preferentially occupied due to the lowered energy state of the 3dxy orbital, which arises from the crystal field asymmetry. We reason that the extra electrons occupy the 3dxy orbital are accumulated at the interface by the displacement of the oxygen atoms. This accumulation contributes to the conductivity of the n-type interface. In addition, through a comparison of the atomic displacements and charge accumulation amounts between the two thickness models (m=3, 5), the thickness-dependency of the conductivity can be explained.

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