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Electronic structures of intrinsic n-type $SrTiO_3$-$LaAlO_3$ interface: density and spatial distribution of free carriers WON-JOON SON, EUNAE CHO, SEUNGWU HAN, Ewha Womans University — The seminal paper by Ohtomo and Hwang reporting the unexpected conductivity when two perovskite insulators, $SrTiO_3$ and $LaAlO_3$, formed an atomically abrupt interface along [001] direction, has aroused an immense interest on the origin of the conductivity. While it is widely accepted that the intrinsic n-type interface is conducting, the carrier density and its spatial distribution are not fully understood. In presentation, first-principles study for establishing the fundamental property of the charge carrier in the intrinsic n-type $LaAlO_3/SrTiO_3$ interface is introduced. To this end, large model systems including up to 20 layers of $SrTiO_3$ and 1–10 layers of $LaAlO_3$ are employed. The charge carrier is observed when $LaAlO_3$ is larger than 3 unit cells and it converges to 0.5 electrons per unit cell. It is also found that the charge carriers transferred from $LaAlO_3$ surface are mostly localized within a few layers from the interface. Furthermore, the electronic states are quantized at the interface with different localization widths, which is similar to electrons in a wedge potential. The carrier density contributed by the interface-localized state shows a good agreement with the experiment.

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