Metal-insulator transition in nanostructured $SrTiO_3/LaAlO_3$

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$SrTiO_3$(STO)/$LaAlO_3$(LAO) heterostructures have attracted significant attention as they exhibit a wealth of intriguing properties such as electric [1], magnetic [2], and superconducting [3] that are absent in their bulk constituents. Among these properties is the presence of a high-mobility two dimensional electron gas (2DEG) when the thickness of the LAO epitaxial layers reaches a critical number of four layers [4]. The requirement of this particular number can be understood by the polar catastrophe" model illustrated in [5], which describes that a minimum number of four LAO layers is needed to accumulate a sufficiently large electric field to enable the transfer of electrons from LAO to the interface [6].

The desired properties of STO/LAO heterostructures depend heavily on novel designs of their atomic structures. For example, nanowire-like STO/LAO heterostructures obtained by the standard photo-lithography technique exhibit a conducting one-dimensional channel [7]. Inspired by this experimental study, we design overlayer heterostructure model formed by combining a LAO overlayer and a regular STO (001) substrate. The stepped LAO surface can be regarded as consisting of an alternating pattern of one and two LAO layers. Therefore, we henceforth refer to this interface as the 1+2 overlayer heterostructure. Figure 1(a) shows a supercell of a the 1+2 STO/LAO overlayer het-erostructure, and Figure 1(b) illustrates the atomic configurations after geometry optimizations. At a regular STO/LAO heterostructure [8], atoms are relaxed primarily along the z direction, whereas at

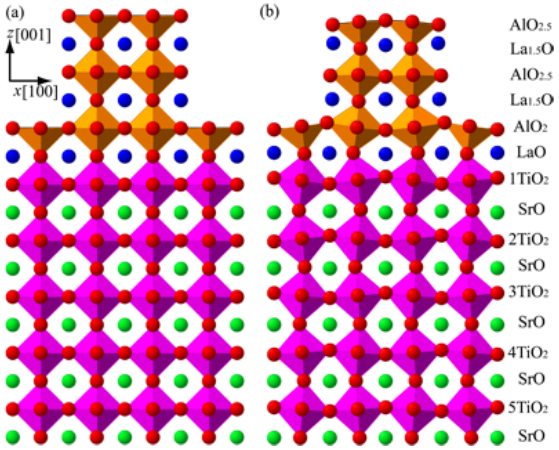

Figure 1. (a) Unrelaxed and (b) relaxed 1+2 STO/LAO overlayer heterostructure. Only one half of the atoms in each supercell are shown. Lanthanum, strontium, and oxygen atoms are illustrated by blue, green, and red balls, respectively. Ti and Al-centered octahedra are represented by magenta and orange polyhedra, respectively. The numbers before the TiO_2 notations denote the order by distance of a TiO_2 layer in STO from the interface.

the overlayer heterostructure, one prominent feature is the rotations of the Ti- and Al-centered octahedra.

In this work, we aim to gain insights on how the peculiar structure, i.e. a STO/LAO overlayer heterostructure affects its electronic properties. Interestingly, we find that metallic states can as well appear at the over-layer heterostructure despite the maximum number of LAO layers is below the aforementioned threshold number. Furthermore, band structures (e.g., see Figure 2) of the overlayer heterostructures show that the metallic states behave as a 2DEG. To this end, we propose a modified polar catastrophe model to understand the occurrence of 2DEGs in these overlayer heterostructures.

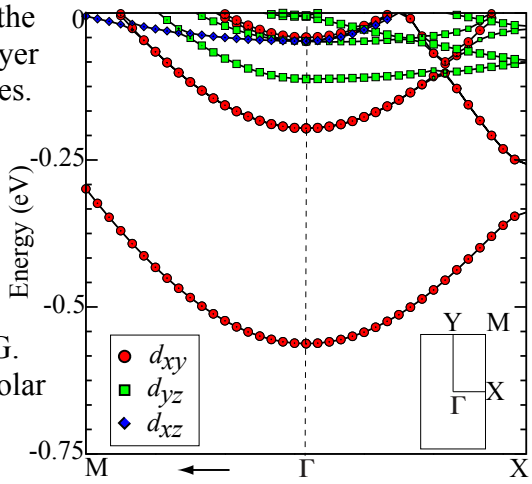

Figure 2. Orbital-resolved band structure of the 1+2 STO/LAO overlayer heterostructure.

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