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The effect of oxygen vacancies on the properties of polar and nonpolar (001) $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures

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ABSTRACT

By using first-principles calculations, we investigated the influence of oxygen vacancy (V_o) on the (001) $\text{LaAlO}_3/\text{SrTiO}_3$ (LAO/STO) heterostructures. Our results show that the effect of V_o on the properties of LAO/STO depends on the polarity of the system. In the polar LAO films V_o screens the internal electric field, which hinders the formation of two-dimensional electronic gas at the interface. V_o cannot reduce the critical thickness of the insulator-to-metal transition although it provides excess electrons. By contrast, in the nonpolar LAO films the metallic states are always maintained regardless of the position of V_o , but V_o causes electronic reconstruction near the Fermi level, and the distribution of conductive electrons differs greatly from the V_o -free case.

Keywords: oxygen vacancy; two-dimensional electronic gas; boundary condition; electronic reconstruction

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