Abstract Submitted
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Two-dimensional electron gasat the interface between two polar oxide materials TULA PAUDEL, EVGENY TSYMBAL, University of Nebraska, Lincoln, NE — Following the discovery of a two-dimensional electron gas (2DEG) at the interface between polar $LaAlO_3$ (LAO) and non-polar $SrTiO_3$ (STO) grown in the [001] direction many related heterostructures with interesting physical phenomena have been proposed and explored. Here using the first-principles theory, we investigate the electronic band structure of the interface between two polar oxide materials – a wide materials group that can broaden the field for designing conducing interfaces with novel properties. As a model system, we consider a LAO/STO heterostructure stacking in the [111] direction. In this direction both free standing LAO and STO are polar with alternatively charged planes – $(LaO_3)^{3-}$ and Al^{3+} in LAO and $(SrO_3)^{4-}$ and Ti^{4+} in STO leading to inevitable interface reconstruction. Simple electrostatic arguments suggest that at the Ti/LaO_3 terminated interface of the LAO/STO(111) heterostructure this reconstruction may be achieved through depositing electron surface charge of $0.5e/\sqrt{3}a^2$ at the interface. This is by a factor of $\sqrt{3}$ smaller than that for the LaO/STO(001) interface which is expected to lead to a larger critical thickness of LAO(111) compared to LAO(001). These arguments are consistent with our first-principles calculations which predict a critical thickness of LAO(111) to be eight (LaO_3-Al) bilayers. Our findings are consistent with the experimental studies performed by S. Ryu, C. W. Bark, T. Hernandez, M. S. Rzchowski, H. Zhou, D. D. Fong, and C.-B. Eom.

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