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First-principles study of $LaAlO_3/SrTiO_3$ thin films KRISTOPHER ANDERSEN, C. STEPHEN HELLBERG, Naval Research Laboratory — Although the perovskite oxides $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) are conventional band insulators, an electron gas can form at their interface. Several mechanisms have been proposed to produce the electron gas, including the electrostatic divergence within LAO that results from the growth of alternating charged $(LaO)^+$ and $(AlO_2)^-$ layers and an electronic reconstruction in which Ti^{3+} and Ti^{4+} is formed at the interface. Of practical interest, thin films of LAO on STO have been observed to have highly mobile carriers and a carrier density that is tunable via LAO thickness—in recent work, Thiel et al. observed an insulator-metal transition between 3–4 MLs. In this talk, first-principles electronic structure calculations are performed on LAO thin films grown on STO to investigate surface reconstructions and the penetration depth of the electron gas into the substrate. An insulator-metal transition is found in good agreement with experiment.

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