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Stoichiometry, defects, and the polar catastrophe in $LaAlO_3$ thin films on $SrTiO_3$ C. STEPHEN HELLBERG, Naval Research Lab — Careful growth of $LaAlO_3$ thin films on $SrTiO_3$ by molecular beam epitaxy has shown that the La/Al ratio of the nominal $LaAlO_3$ layer is key to the formation of a two-dimensional electron liquid at the interface—metallic conductivity is only observed in Al-rich films. The interfacial electron liquid forms due to the polar catastrophe, the diverging potential caused by the atomic layer arrangement at the interface when polar $LaAlO_3$ is grown on TiO_2-terminated non-polar $SrTiO_3$. The system eventually reconstructs, moving negative charges to the interface to screen the diverging potential. I will present density functional calculations of the defects that form in $LaAlO_3$ on $SrTiO_3$ to accomodate variations in stoichiometry. In La-rich films, the lowest energy defects are extended and allow cation vacancies to move to the interface to screen the diverging potential. Thus the interface between La-rich $LaAlO_3$ and $SrTiO_3$ remains insulating. In Al-rich films, the defects are localized and block cation motion. In this case a conducting electron liquid forms to screen the diverging potential.

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