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Importance of the surface in interfacial conductivity in LaAlO₃ thin films on SrTiO₃ C. STEPHEN HELLBERG, Naval Research Lab — Careful growth of LaAlO₃ thin films on SrTiO₃ by molecular beam epitaxy has shown that the La/Al ratio of the film 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 LaAlO₃ is grown on TiO₂-terminated non-polar SrTiO₃. The system eventually reconstructs, moving negative charges to the interface to screen the diverging potential. I will present density functional calculations showing the defects that form in the film depend on the stoichiometry, and these defects lead to electronic reconstruction in Al-rich films and ionic reconstruction in La-rich films. The stoichiometry of the surface differs from that the bulk of the film, and I will show that the LaAlO₃ surface is unstable to phase separation. The interaction between surface and bulk leads to a scenario where the insulating La-rich films have an Al-rich surface.

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