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Role of stoichiometry in the interfacial metal-insulator transition in $LaAlO_3/SrTiO_3$ C. STEPHEN HELLBERG, Naval Research Laboratory & Center for Nanoscale Science and Technology, NIST, KRISTOPHER ANDERSEN, High Performance Technologies, Inc. & Naval Research Laboratory — The observed metal-insulator transition in thin films of $LaAlO_3$ on $SrTiO_3$ depends critically on the stoichiometry of the film: metallic interfaces are found for Al-rich films, while growing even slightly La-rich films results in insulating interfaces. Using first-principles density functional calculations, we examine the effects of changing the stoichiometry of the films. We find that Al will substitute for La, but La will not substitute for Al. Instead, the excess La sits on the surface of the film. The combination of Al vacancies in the film and excess La on the surface screens the diverging electrostatic potential responsible for forming a metallic interface.

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