

Abstract Submitted
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Importance of defects and stoichiometry in the interfacial metal-insulator transition in LaAlO₃ thin films on SrTiO₃ C. STEPHEN HELLBERG, Naval Research Lab — The observed metal-insulator transition in thin films of LaAlO₃ on SrTiO₃ depends critically on the stoichiometry of the film: metallic interfaces are found for Al-rich films, while growing even slightly La-rich 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, Al-vacancy structures occur in La-rich films. The Al vacancies can migrate to the interface, screening the potential divergence and preventing a metallic interface from forming.

C. Stephen Hellberg
Naval Research Lab

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