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Theory of the Switchable Interfacial Metal-Insulator Transition in LaAlO₃ thin films on SrTiO₃ C. STEPHEN HELLBERG, Naval Research Lab, KRISTOPHER ANDERSEN, Northern Arizona University, CHENG CEN, JEREMY LEVY, University of Pittsburgh, STEFAN THIEL, GERMAN HAMMERL, CHRISTOF SCHNEIDER, JOCHEN MANNHART, Augsburg University — Although bulk LaAlO₃ and SrTiO₃ are both insulating, an electron gas can form at the interface between these compounds. For up to 2 unit cells (uc) of LaAlO₃, the interface remains insulating, while for 4 uc and beyond, it is metallic. For 3 uc films, the interface can be reversibly switched from metallic to insulating using voltages applied by an atomic force microscope (AFM). We present first- principles density functional calculations of LaAlO₃ films on SrTiO₃. We show the AFM induced interfacial metal- insulator transition can be explained by the formation and annihilation of oxygen vacancies on the LaAlO₃ surface.

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