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Oxygen vacancies at the $LaAlO_3/SrTiO_3$ interface: formation energies and metal-insulator transition HANGHUI CHEN, Department of Physics, Yale University, ALEXIE KOLPAK, Department of Material Science and Engineering, MIT, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — The intriguing transport properties observed at the $LaAlO_3/SrTiO_3$ interface have stimulated numerous studies in the past few years. However, the microscopic mechanism that leads to the formation of the two-dimensional conducting electron gas at the interface remains elusive, partly due to the fact that both intrinsic and extrinsic factors can contribute. We report first principles results on the formation energies of oxygen vacancies on the $LaAlO_3$ thin film surface as a function of coverage and film thickness. In addition to electrostatic contributions to the formation energy due to the polar field in $LaAlO_3$, structural distortions also play an important role in the energetics. We build a simple analytical model to describe our findings which allows us to determine the critical thickness for an oxygen vacancy-induced metal-insulator transition. We discuss the relation of these predictions to the experimental results on this interfacial system.

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