Intermixtures at $LaAlO_3/SrTiO_3$ interfaces

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The intriguing transport properties observed at the $LaAlO_3/SrTiO_3$ n-type interface have precipitated numerous studies in the past few years. However, it remains uncertain whether the interface obtained experimentally is atomically sharp, and if not, what role the disorder plays in the unique behavior of this system. We use first principles density functional theory to find the energetics of cation intermixing, specifically La-Sr and Al-Ti, at the $LaAlO_3/SrTiO_3$ n-type interface. We find that an ideal interface with no intermixing is not thermodynamically stable. Ti-Al intermixing reduces the total energy while Sr-La intermixing increases the total energy. We explain the energetics and this asymmetry in terms of a simple electrostatic model, which is able to accurately describe the DFT results. We also discuss how intermixing affects the polar field in the $LaAlO_3$, the "polar catastrophe", and the critical thickness of $LaAlO_3$ needed to induce a metal-insulator transition.