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Polarity compensation mechanisms in LaAlO_3 (001) - oriented thin films HOSUNG SEO, ALEXANDER DEMKOV, Department of Physics, The University of Texas at Austin — Lanthanum aluminate LaAlO_3 (LAO) is a polar perovskite oxide widely used as a substrate in oxide epitaxy. Thin films of LAO are of particular interest in view of a recent discovery of the two-dimensional electron gas at the $\text{LaAlO}_3/\text{SrTiO}_3$ interface. In the (001) direction, the LAO thin film can be regarded as a stack of alternating charged LaO and AlO_2 planes. Therefore, an unreconstructed LAO thin film would have a macroscopic electric field built up and is expected to have a highly unstable surface. In this talk, we discuss theoretically possible microscopic surface reconstructions compensating the electric field. We use the density functional theory approach within the local density approximation. We find that lanthanum vacancies on the LaO-terminated surface or oxygen vacancies on the AlO_2 -terminated surface can effectively compensate the electric field in the LAO(001) thin films.

Hosung Seo
Department of Physics, The University of Texas at Austin

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