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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 LaAlO$_3$/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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