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Understanding polarity compensation across polar LaAlO₃ films

G. SINGH-BHALLA, LBL, UC Berkeley, P. ROSSEN, UCB, S. JAGANATH, G. PALSSON, D. YI, LBL, A. DASGUPTA, J. RAVICHANDRAN, UCB, V. RUIZ, U Munich, J. HERON, UCB, C. FADLEY, LBL, A. YADAV, UCB, R. PENTCHEVA, U Munich, R. RAMESH, UCB, LBL — Dipole screening mechanisms for polar crystals can manifest in a variety of ways depending on bandgaps, surface energies and environmental conditions. Here we study the polarity compensation process in LaAlO₃ thin film grown on the two different surface terminations of [001] SrTiO₃ crystals (SrO and TiO₂). An electron gas that appears at the interface between LaAlO₃ and TiO₂-SrTiO₃ surface (n-type) potentially screens the LaAlO₃ polarity, while the interface between LaAlO₃ and SrO-SrTiO₃ (p-type) remains insulating. To understand this asymmetry, we probed the LaAlO₃ surface using a variety of element-specific probes and observe a change in the LaAlO₃ stacking structure in the p-type geometry. Tunneling measurements reveal remnants of a built-in field reflective of LaAlO₃'s intrinsic polarity across the n-type structure, but no such signatures are detected for the p-type structure. When combined with density functional theory simulations, the results suggest that while free charge screens the LaAlO₃ dipole in the n-type geometry, a change in LaAlO₃'s structure during growth nullifies the dipole in the p-type geometry. In essence, SrTiO₃ surface layers drastically affect LaAlO₃ polarity compensation and in turn the electronic properties.

Guneeta Singh-Bhalla
LBL, UC Berkeley

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