

Abstract Submitted  
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**Electronic structure and stability of  $\text{LaAlO}_3$  surfaces using first-principles calculations**<sup>1</sup> KARTHIK KRISHNASWAMY, CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, Univ of California - Santa Barbara —  $\text{LaAlO}_3$  (LAO) is a wide-band gap complex oxide that is often used as a substrate in the growth of other oxides, and has been considered as a high- $k$  gate dielectric for CMOS devices. In addition, a high-density two-dimensional electron gas (2DEG) at the interface between LAO and  $\text{SrTiO}_3$  (STO) has been observed, showing strong dependence on surface termination and on the thickness of the LAO top layer. The possibility of tuning the 2DEG has triggered the interest in these heterostructures for electronic devices. In all of these applications, the surface of LAO is expected to play a key role, yet its electronic structure and surface stability are poorly understood. Using first-principles calculations based on hybrid density functional theory, we determine the low-energy (001) terminations of LAO and their reconstructions. We analyze the surface stability as a function of oxygen chemical potential and relate to experimental conditions. We discuss the case of bulk single crystals in which the electric field inside the material can be neglected, and also the case of LAO thin films on STO, in which the surface stability can be affected by the presence of the 2DEG at the STO/LAO interface.

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