Abstract Submitted
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Stability and electronic structure of $GdTiO_3$ surfaces[1] KARTHIK KRISHNASWAMY, University of California, Santa Barbara , ANDERSON JANOTTI, University of Delaware, LARS BJAALIE, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — $GdTiO_3$ (GTO) is a Mott insulator with the Ti atoms in a +3 oxidation state. Similar to the extensively studied $LaAlO_3/SrTiO_3$ (LAO/STO), the GTO/STO (001) interface also exhibits a polar discontinuity that results in the formation of a high-density two-dimensional electron gas (2DEG). However, in contrast to the LAO/STO system, where the LAO surface strongly influences the 2DEG properties and causes an LAO-thickness dependence of the 2DEG density; the surface termination of GTO does not affect the 2DEG properties at the GTO/STO interface. Using first-principles calculations, we examine the surface properties of LAO and GTO, and determine their impact on the 2DEG properties. We find that the energetic positions of surface states in LAO and GTO explain the differences in their impact on the 2DEG. In addition, we find that the polar TiO_2 surface termination of GTO is very stable, with a low surface energy, even compared to a hydrogenated surface. The TiO_2termination is insulating, while the GdO termination is found to be metallic. Our results shed light on the peculiar behavior of the polar surfaces of Mott insulators in general.

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