

Abstract Submitted
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Band alignments at the interface of complex oxides¹ LARS BJAALIE, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California Santa Barbara — The realization of a two-dimensional electron gas at the SrTiO₃/LaAlO₃ interface has spurred interest in the development of electronic devices based on complex oxides. In the design of such devices it is crucial to know the band alignment at the interface of the different oxides, a key quantity that governs carrier barrier heights and carrier confinement. Reported values for the valence-band alignment at the SrTiO₃/LaAlO₃ interface vary by more than 1 eV. Using first-principles calculations based on a hybrid functional we calculate the band alignment at the interface between various complex oxides, including the band insulators SrTiO₃, SrZrO₃, LaAlO₃, CaTiO₃, and GaAlO₃ and the Mott insulators GdTiO₃ and YTiO₃. This choice of materials allows us to analyze the effects of cation size, lattice parameters, band gaps, and lattice orientation on the band alignment.

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