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Evolution of the Band Alignment at Polar Oxide Interfaces J.D. BURTON, EVGENY TSYMBAL, University of Nebraska - Lincoln — The next generation of electronic devices and systems are envisioned to exploit the multifunctional properties of complex oxide interfaces. Fundamental to this endeavor is an understanding of the electronic band alignment across such interfaces. Engineering this band alignment in all-oxide systems by properly preparing the interfaces is highly desirable. Here we explore an all-oxide metal-insulator interface between, $SrTiO_3$ (STO), and $La_{1-x}A_xMnO_3$ (LAMO), where A is a divalent cation [1]. The doping level of the manganite, x, offers a parameter which can be varied to engineer the band alignment. We use first-principles density-functional calculations to determine the evolution of the band alignment at $La_{0.7}A_{0.3}MnO_3|La_{1-x}A_xO|TiO_2|SrTiO_3(001)$ heterointerfaces as the interfacial composition, $La_{1-x}A_x$, is varied. The position of the valence band maximum (VBM) with respect to the Fermi level increases linearly with interfacial composition x due to the linear dependence of the screened electrostatic interface dipole on the interfacial ionic charge. The importance of the polar nature of LAMO and its background dielectric properties will be discussed. Our results are agreement with recent experimental data reported by Hikita *et al* [2].
[1] J. D. Burton and E. Y. Tsymbal, Phys. Rev. B 82, 161407 (2010).
[2] Y. Hikita *et al.*, Phys. Rev. B 79, 073101 (2009).

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