Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Band alignments at oxide interfaces and consequences for devices CHRIS VAN DE WALLE, LARS BJAALIE, BURAK HIMMETOGLU, Univ of California - Santa Barbara, LEIGH WESTON, Univ of Sydney, ANDERSON JANOTTI, Univ of California - Santa Barbara — Oxide heterostructures have been shown to exhibit unusual physics and hold the promise of novel electronic applications. We present a set of criteria to select and design interfaces, particularly those that can sustain a high-density two-dimensional electron gas (2DEG). We describe how first-principles calculations, based on hybrid density functional theory, can contribute to a qualitative and quantitative understanding, illustrated with the key issue of band alignment. Band offsets determine on which side of the interface the 2DEG will reside, as well as the degree of confinement. We present band alignments for a number of complex oxides, considering materials with different types of conduction-band character, polar or nonpolar character, and band insulators as well as Mott insulators. We suggest promising materials combinations that could lead to a 2DEG with optimized properties, such as high 2DEG densities and high electron mobilities.

Chris Van de Walle
Univ of California - Santa Barbara

Date submitted: 15 Nov 2013 Electronic form version 1.4