MAR14-2013-020224

Abstract for an Invited Paper
for the MAR14 Meeting of
the American Physical Society

Controlling the two-dimensional electron gas at complex oxide interfaces[1]

ANDERSON JANOTTI, University of California Santa Barbara

Heterostructures of complex oxides have attracted great interest since the demonstration of a high-density two-dimensional electron gas (2DEG) at the $SrTiO_3/LaAlO_3$ (STO/LAO) interface. Still, the density of the 2DEG is only one tenth of what was expected from simple electron counting, i.e., 1/2 electron per unit-cell area. Since then, the origin and amount of the charge, the electrical properties of the 2DEG, the role of native defects, and the abrupt variation of the electron density with the thickness of the LAO top layer have been the subject of numerous theoretical and experimental studies. More recently, a 2DEG with the full density of 1/2 electron per unit cell area has been observed at the interface between the band insulator STO and the Mott insulator $GdTiO_3$ (GTO) [1], shedding additional light on the origin of the 2DEG, and raising important questions on the differences between the STO/LAO and STO/GTO heterostructures. Here we will discuss the similarities of the 2DEG at the STO/LAO and STO/GTO heterostructures from the perspective of first-principles simulations. We will address the differences in band alignments in the STO/LAO and STO/GTO heterostructures, and how the 2DEG is affected by the surface of the LAO top layer in the STO/LAO, but apparently not in the STO/GTO case [2]. Finally, we will also discuss how heterostructures can be used to drastically alter the electronic structure of STO, transforming it from a band insulator into a Mott insulator.

[1] P. Moetakef, T. A. Cain, D. G. Ouellette, J. Y. Zhang, D. O. Klenov, A. Janotti, C. G. Van de Walle, S. Rajan, S. J. Allen, and S. Stemmer, App. Phys. Lett. **99**, 232116 (2011).
[2] A. Janotti, L. Bjaalie, L. Gordon, and C. G. Van de Walle, Phys. Rev. B **86**, 241108(R) (2012).

[1]This work was performed in collaboration with Lars Bjaalie, Luke Gordon, Burak Himmetoglu, and Chris G. Van de Walle, and supported by ARO and NSF.