

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Evolution of the electronic structure of SrTiO<sub>3</sub>/GdTiO<sub>3</sub> heterostructures with layer thickness** LARS BJAALIE, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — A two-dimensional electron gas (2DEG), with density of  $3 \times 10^{14} \text{cm}^{-2}$  (0.5 electrons per interface unit cell), has been observed at the SrTiO<sub>3</sub>/GdTiO<sub>3</sub> interface, with potential applications in electronic devices [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, Appl. Phys. Lett. 99, 232116 (2011)]. Yet, basic properties of the 2DEG is still poorly understood, in particular the variation of the electrical conductivity with the SrTiO<sub>3</sub> layer thickness. We performed density functional calculations with a hybrid functional to study the electronic structure of SrTiO<sub>3</sub>/GdTiO<sub>3</sub> superlattices. We address the insulator to metal transition as a function of layer thickness, analyzing the effects of quantum confinement, charge ordering, and lattice distortions. Work supported by NSF and ARO.

Lars Bjaalie  
University of California, Santa Barbara

Date submitted: 15 Nov 2013

Electronic form version 1.4