

HL 14: Invited Talk: Chris van de Walle

Time: Monday 13:30–14:00

Location: H2

Invited Talk

HL 14.1 Mon 13:30 H2

Complex oxides for next-generation electronics — •CHRIS G. VAN DE WALLE — Materials Department, University of California, Santa Barbara, USA

The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, SrTiO₃ (STO) and LaAlO₃ (LAO), has sparked huge interest in oxide electronics. The mechanisms that determine the density of this 2DEG have not yet been unravelled. The polar discontinuity at the STO/LAO interface can in principle sustain an electron density of $3.3 \times 10^{14} \text{ cm}^{-2}$ (0.5 electrons per unit cell), but experimentally observed densities are more than an order of magnitude lower. We have used a combination of first-principles calculations and Schrödinger-Poisson simulations to investigate the origin

of the electrons in the 2DEG at the STO/LAO interface. We find that the inability to form a symmetric set of interfaces limits the 2DEG density [1]. The effects of different terminations of the LAO surface are examined. Our results apply to oxide interfaces in general, and explain why the SrTiO₃/GdTiO₃ interface has been found to exhibit the full density of 0.5 electrons per unit cell [2].

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[1] A. Janotti, L. Bjaalie, L. Gordon, and C. G. Van de Walle, Phys. Rev. B 86, 241108(R) (2012).

[2] 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).