

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

### **Tuning**

**the two-dimensional electron gas at the  $\text{LaAlO}_3/\text{SrTiO}_3(001)$  interface by metallic contacts**<sup>1</sup> ROSSITZA PENTCHEVA, REMI ARRAS, VICTOR G. RUIZ LOPEZ, Ludwig Maximilians University Munich, Germany, WARREN E. PICKETT, University of California, Davis — Density functional theory calculations reveal that adding a metallic overlayer on  $\text{LaAlO}_3/\text{SrTiO}_3(001)$  reduces/eliminates the electric field within the polar  $\text{LaAlO}_3$  film and thus suppresses the thickness-dependent insulator-to-metal transition observed in uncovered films. Independent of the  $\text{LaAlO}_3$  thickness both the surface and the interface are metallic, with an enhanced interface carrier density relative to  $\text{LaAlO}_3/\text{SrTiO}_3(001)$  after the metallization transition. Moreover, a monolayer thick metallic Ti-contact exhibits a finite magnetic moment and for a thin  $\text{SrTiO}_3$ -substrate induces a spin-polarized 2D electron gas at the  $n$ -type interface due to confinement effects. The height of the Schottky barrier formed between the metal contact and  $\text{LaAlO}_3$  depends strongly on the choice of the overlayer and allows to tune the carrier density at the interface [1].

[1] V. Ruiz López, R. Arras, W. E. Pickett, and R. Pentcheva, arXiv:1106.4205v1.

<sup>1</sup>Funding by the DFT, SFB/TR80 is gratefully acknowledged.

Rossitza Pentcheva  
Ludwig Maximilians University Munich, Germany

Date submitted: 13 Dec 2011

Electronic form version 1.4