Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Band-alignment issues in the *ab initio* simulation of ferroelectric nanocapacitors PABLO AGUADO-PUENTE, CITIMAC, Universidad de Cantabria, los Castros s/n, 39005 Santander, Spain, MASSIMILIANO STENGEL, NICOLA SPALDIN, Materials Department, University of California, Santa Barbara, CA 93106-5050, USA, JAVIER JUNQUERA, CITIMAC, Universidad de Cantabria, los Castros s/n, 39005 Santander, Spain — Recent advances in growing and characterization techniques of complex oxides thin films have lead to the development of many novel interface-based devices with a great number of new functionalities, such as the formation of 2D electron gases or spin-polarized tunnel junctions. These experimental developments have been accompanied by a great explosion of theoretical works aiming to understand the origin of such phenomena. DFT simulations, both within LDA or GGA aproximations, have been shown to be an extremely powerful tool to study these systems. However, it is important to identify, in adition to the virtues, also the limitations of DFT which are specific to metal/perovskite interfaces, and that when overlooked might lead to erroneous physical conclusions. In this work we study the consecuences of the band-gap underestimation by usual DFT functionals. We show how this underestimation might lead to wrong band alignments both in nonpolar and in polar complex oxides heterostructures, and how they give rise to unphysical charge transfers across the interfaces. We also provide analysis tools to detect the fingerprints of such pathological behaviour.

Pablo Aguado-Puente
Universidad de Cantabria

Date submitted: 20 Nov 2009 Electronic form version 1.4