Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Two-dimensional electron gases at head-to-head and tail-to-tail domain walls in ferroelectric thin films.[1] PABLO GARCíA-FERNÁNDEZ, Universidad de Cantabria, JORGE ÍÑIGUEZ, Luxembourg Institute of Science and Technology, JAVIER JUNQUERA, Universidad de Cantabria — Symmetry breaking at ferroelectric domain walls gives rise to new physical properties, offering the opportunity to use the domain walls themselves as a functional separate object in a device. One example is the appearance of an enhanced conductivity at the boundaries between ferroelectric domains in oxides. A realistic first-principles simulation of the domains walls is limited to highly-symmetric cleanly-cut walls in order to keep the number of atoms in the simulation box small. Here we use a recently developed second-principles method that treats all the lattice degrees of freedom and the relevant electronic ones on the same foot with high accuracy at a modest computational cost. We apply it to the demading physical problem of head-to-head (HH) and tail-to-tail (TT) domain walls in ferroelectric $PbTiO_3$ thin films. These interfaces present a large and unfavourable electrostatic energy due to the polarization-induced bound charge at the domain wall. An accurate simulation should capture eventual charge transfers between the walls, and the concomitant electron-lattice coupling. We show how the polarization discontinuity in HH and TT domain walls in $PbTiO_3$ thin films can be effectively screened by the formation of two-dimensional electron gases of electrons and holes.

[1]Finantial support from MINECO Grant No. FIS2012-37549-C05-04

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Date submitted: 06 Nov 2015 Electronic form version 1.4