Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Polarization scaling in ultrathin epitaxial ferroelectric heterostructures: First-principles results JAVIER JUNQUERA, Dep. of Physics and Astronomy, Rutgers University,Piscataway, NJ 08854-8019, PHILIPPE GHOSEZ, Dép. de Physique, Université de Liège, B-4000 Sart-Tilman, Belgium, KARIN M. RABE, Dep. of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019 — To resolve the apparent inconsistency between the high c/a and the low measured switchable polarization of ultrathin $Pb(Zr_{0.2}Ti_{0.8})O_3$ (PZT) films [1], we have carried out first-principles effective hamiltonian simulations. The epitaxial strain constraints and the thickness dependent residual depolarization field $\mathcal{E}_d$, arising from an incomplete screening of the dipole surface density by real metallic electrodes, [2] are properly included. As the thickness decreases below 150Å, the increase of $\mathcal{E}_d$ in the uniformly polarized state drives a phase transition to a state with 180^o stripe domains, similar to that observed for $PbTiO_3$ films on insulating substrates [3]. Although the net polarization is zero, each domain exhibits the bulk strained polarization and tetragonality, 1.25 % larger than in the unstrained sample, yielding a consistent interpretation of the experimental data. Work supported by DOE Grant DE-FG02-01ER45937

[1]V. Nagarajan *et al.*, previous abstract
[2]J. Junquera and Ph. Ghosez, Nature **422**, 506 (2003)
[3]D. D. Fong *et al.*, Science, **304** 1650 (2004)

Javier Junquera
Dep. of Physics and Astronomy, Rutgers University,Piscataway, NJ 08854-8019

Date submitted: 01 Dec 2004 Electronic form version 1.4