Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Theoretical study of ferroelectric switching of $Pt/BaTiO_3$ Slabs KURT FREDRICKSON, ALEX DEMKOV, The University of Texas at Austin — $BaTiO_3$(BTO) is a well known ferroelectric perovskite, which is tetragonal at room temperature. The energy barrier for polarization switching is small at 9.7 meV; however, its energy barrier clamped between two metal electrodes is an open question. It has been shown (Junquera & Ghosez, Nature **422**, 506 (2003)) that the ferroelectric behavior is highly thickness dependent. We examine thin slabs of BTO sandwiched between electrodes of Pt and calculate the polarization barriers using density functional theory to see whether the barrier should be surmountable. We have found that the energy barrier/unit cell reaches the bulk value at only 10 unit cells of BTO. We also examine the polarization of the relaxed slabs and compare them to bulk BTO, and find that the center of the slab exhibits bulk rumpling at 20 unit cells of BTO.

Kurt Fredrickson
The University of Texas at Austin

Date submitted: 20 Nov 2011 Electronic form version 1.4