Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Ab initio **calculations of $BaTiO_3$, $PbTiO_3$ and $SrTiO_3$ (001) and (011) surfaces** ROBERTS EGLITIS, DAVID VANDERBILT, Rutgers University, RUTGERS UNIVERSITY TEAM — We present results of calculations of surface relaxations and rumplings[1] for the (001) and (011) surfaces of $ATiO_3$ perovskites (A=Ba, Pb, and Sr) using a hybrid B3PW description of exchange and correlation. On the (001) surfaces, we consider both AO and TiO_2 terminations. In the former case, the surface AO layer is found to relax inward for all three materials, while outward relaxations of all atoms in the second layer are found for both kinds of (001) terminations. The surface relaxation energies of AO and TiO_2 terminations are found to be comparable with each other for all three materials. For (011) surfaces, we consider terminations on a TiO layer, an A layer, or an O layer. The surface relaxation energies for $BaTiO_3$, $PbTiO_3$ and $SrTiO_3$ (011) surfaces for all terminations are considerable larger than for (001) surfaces. Among the (011) surfaces, the relaxation energy is much larger for the TiO-terminated surface than for the Ba- or Pb-terminated surfaces for the $BaTiO_3$ and $PbTiO_3$ perovskites. We predict a considerable increase in the Ti-O chemical bond covalency near the (011) surfaces as compared to both the bulk and the (001) surfaces.

[1]R. I. Eglitis and D. Vanderbilt, Phys. Rev. B **76**, 155439 (2007).

Roberts Eglitis
Rutgers University

Date submitted: 20 Nov 2007 Electronic form version 1.4