Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles prediction of switchable stoichiometry at interfaces SERGEY V. LEVCHENKO, ANDREW M. RAPPE, University of Pennsylvania — We present a first-principles density functional theory (DFT) study of the relative thermodynamic stability of ferroelectric (FE) lithium niobate ($LiNbO_3$) (0001) surfaces of different stoichiometry. We predict that the equilibrium stoichiometries are different for the positively and negatively polarized $LiNbO_3$ surfaces under the same conditions. A correct way of calculating surface charges for ferroelectric materials with intrinsic polar stacking is developed. It is found that surface charge passivation by ions is thermodynamically favored over passivation by mobile carriers in a wide range of chemical potentials.

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Date submitted: 27 Nov 2007 Electronic form version 1.4