Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Structure and energetics of ferroelectric domain walls in $LiNbO_3$ from atomic level simulations[1] DONGHWA LEE, Lawrence Livermore National Laboratory, HAIXUAN XU, Oak Ridge National Laboratory, VOLKMAR DIEROLF, Lehigh University, VENKATRAMAN GOPALAN, Pennsylvania State University, SIMON PHILLPOT, University of Florida, UNIVERSITY OF FLORIDA TEAM, LEHIGH UNIVERSITY COLLABORATION, PENNSYLVANIA STATE UNIVERSITY COLLABORATION — Due to its unique ferroelectric and nonlinear optical properties, $LiNbO_3$ has a wide range of applications in optoelectronics and nonlinear optics. These unique properties of $LiNbO_3$ are, however, quite sensitive to point defects and ferroelectric domain walls. Therefore, detailed characterization of the ferroelectric domain walls and their interaction with the defects at atomistic scale is highly important The local structure and energetics of the ferroelectric domain walls in $LiNbO_3$ are examined using density functional theory (DFT) and atomistic-level simulation methods. The energetics and electric dipoles associated with the pertinent point defects and domain walls in $LiNbO_3$ are investigated in detail. In particular, the variation of polarization due to 180° ferroelectric domain walls, the coupling of defect-domain wall interactions and their effects on domain wall motion are discussed

[1]This work was supported by NSF under Materials World Network Grant Number DMR-0602986, DMR-0908718, and DMR-0820404.

Donghwa Lee
Lawrence Livermore National Laboratory

Date submitted: 19 Nov 2010 Electronic form version 1.4