Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

**Internal electric field effects in ferroelectric nanostructures**[1] BYOUNGHAK LEE, ZHENGJI ZHAO, LIN-WANG WANG, Lawrence Berkeley National Lab — A ground state dipole moment of ferroelectric nanostructures is a long-standing problem. A permanent dipole moment can alter optical and electronic properties of nanostructures, causing state localizations and electron hole separations. A dipole moment in the bulk can have a self-screening effect. In a nanostructure, the different shape of the system can result in an effective screening different from the bulk. In ferroelectric nanostructures, this can lead to a shape dependent total dipole moment, different from the volumetric result derived from its bulk value. Direct ab initio theoretical study on the nanostructure dipole moment is scarce due to the large computational cost. We present a first principles study of this problem using a recently developed Linear Scaling 3-Dimensional Fragment method. We investigated shape and size dependence of the surface and bulk contributions of the electric dipole moment in various ferroelectric nanorods. We compared our results with experiments and provided an insightful physical picture by analyzing the ab initio numerical results with a classical dielectric model.

[1]This work is supported by DOE/BES, DE-AC02-05CH11231. It used the resources of National Center for Computational Sciences (NCCS) and National Energy Research Scientific Computing Center (NERSC).

Byounghak Lee
Lawrence Berkeley National Lab

Date submitted: 27 Nov 2007 Electronic form version 1.4