Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Multi-scale Simulation of Ferroelectric Properties in Perovskite Solid YAJIE LEI, George Washington University, JAMES LEE, YOUPING CHEN, LIMING XIONG — The first principles calculations provide us with the fundamental information for the study of ferroelectric materials, including the atomic structures of morphotropic phases, ferroelectric double-well potentials, dynamical effective charges and phonon spectra. Building on such information obtained from the electronic-structure calculations by density functional theory, we developed a multi-scale approach with parameterization of the classical Buckingham potential. Applying the empirical potentials to the atomistic modeling method and a newly developed continuum theory, the ferroelectric behaviors of BiScO3 are investigated through dynamical simulations. This approach illustrates the capability to study ferroelectric materials with finite temperature and external electromechanical loadings, with no limitation to a small system with zero temperature as being imposed in the first principles calculations.

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Date submitted: 30 Nov 2005 Electronic form version 1.4