Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principles calculation of phonon dispersions for $\mathbf{Ba_{1-x}Ca_xTiO_3}$[1] TAICHI KOSUGI, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo — Amongst perovskite oxides, $BaTiO_3$(BTO) is widely used for its distinct dielectric, piezoelectric and optical properties. Its lattice dynamics, associated with atomic displacements, have been intensively studied both theoretically and experimentally, since is essential for the dielectric instability of this material. Recently Ca-doped BTO(BCTO) single crystal was synthesized by Fu et al. and found to have exotic natures. Using the direct method proposed by Parlinski, we calculated the phonon dispersions of BCTO in a fully *ab initio* manner, in which the force constants, the Born effective charges and the dielectric tensors are determined from first-principles.

[1]This work was supported by the Next Generation Super Computing Project, Nanoscience Program, MEXT, Japan.

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Date submitted: 27 Nov 2007 Electronic form version 1.4