Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Local Basis Set Supercell Studies of (K,Na)NbO$_3$ Solid Solutions
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Oak Ridge National Laboratory — We report density functional supercell calculations for (K,Na)NbO$_3$ perovskite solid solutions using the local basis SIESTA code. We did detailed comparisons of results for ferroelectric structures and vibrational frequencies obtained with SIESTA with those obtained using all-electron full potential LAPW calculations, and used these comparisons to establish compact but accurate choices of basis set and pseudopotentials for the SIESTA calculations. Supercell calculations using SIESTA are used to investigate the dependence of ferroelectric polarization and local structure on the K/Na ordering. This work was supported by the DOE ORNL LDRD program and the Office of Naval Research.

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Date submitted: 17 Nov 2006