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Local Basis Set Supercell Studies of (K,Na)NbO₃ Solid Solutions RICARDO KAGIMURA, MALLIGA SUEWATTANA, DAVID J. SINGH, Oak Ridge National Laboratory — We report density functional supercell calculations for (K,Na)NbO₃ 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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