Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Dielectric properties of the $BaTiO_3 - Bi(Zn_{\frac{1}{2}}Ti_{\frac{1}{2}})0_3$ solid solution from density-functional theory DENNIS JACKSON, DAVID ROUNDY, Oregon State University — Using density functional theory combined with the modern theory of polarization, we predict dielectric properties of $BaTiO_3$ and $Bi(Zn_{\frac{1}{2}}Ti_{\frac{1}{2}})0_3$ in solid solution. In particular, we study the effects of disorder on the system in the presence of a homogeneous finite electric field. We consider all unique configurations of the solid solution in a given supercell, computing the polarization resulting from a given applied field. This provides a statistical ensemble from which we predict the finite-temperature dielectric response. We will discuss the implications for uniform bulk solids and within polar nano-regions of a non-uniform solid.

Dennis Jackson
Oregon State University

Date submitted: 19 Nov 2009 Electronic form version 1.4