Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Origin of Curie temperature non-linearity in ferroelectric $BiBO_3$-$PbTiO_3$ solid solutions ILYA GRINBERG, Department of Chemistry, University of Pennsylvania, ANDREW M. RAPPE, Department of Chemistry, University of Pennsylvania — We use first-principles density functional theory calculations to investigate compositional trends in ferroelectric $BiBO_3$-$PbTiO_3$ solid solutions. We find that cation displacements which give rise to ferroelectricity in these materials follow a linear relationship with the average displacive characteristics of the B-site. The transition temperatures in these materials are well correlated with polarization magnitudes computed from our calculations. The coupling between composition of the B-site and A- and B-site displacements explains the highly nonlinear and sometimes non-monotonic dependence of the Curie temperature (T_c) on composition observed in these materials.

Ilya Grinberg
Department of Chemistry, University of Pennsylvania

Date submitted: 30 Nov 2005 Electronic form version 1.4