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Multi-scale Modeling of Relaxor Ferroelectrics ARAVIND ASTHAGIRI, Carnegie Institution of Washington, NARAYANI CHOUDHURY, Bhabha Atomic Research Centre, WU ZHIGANG, RONALD COHEN, Carnegie Institution of Washington — The origin of the high piezoelectric response observed in complex solid solution perovskites like $PbMg_{1/3}Nb_{2/3}O_3$-$PbTiO_3$ (PMN-PT) is still not well understood. We have taken a multi-scale approach to examine PMN and PMN-PT by developing a shell potential model by fitting to extensive first-principles data that can then be used in molecular dynamics (MD) simulations. For PMN we have performed both total energy calculations with LAPW and linear response calculations using ABINIT to obtain the phonon spectra of ordered 1:2 supercells along the [111] and [001] directions. For both ordered structures, we find small energy differences between the polar ferroelectric and non-polar antiferroelectric structures and large LO-TO splittings. For the [111] structure, we find the ground state to be triclinic. The results above and similar results for $PbTiO_3$ have been used to fit a shell model potential for PMN and PT. We will report the temperature and applied field behavior of disordered PMN and the phase diagram of PMN-PT obtained from MD simulations and compare to existing experimental data. Preliminary results for PMN indicate that we obtain qualitatively similar Raman spectra and bulk modulus to experiment. Work supported by the Office of Naval Research (contract number N000149710052) and the Carnegie Institution of Washington.

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