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Molecular dynamics computational studies of relaxor ferroelectric behavior in $Pb(Mg_{1/4}Ti_{1/4}Nb_{1/2})O_3$ (PMN-PT) HIROYUKI TAKENAKA, ILYA GRINBERG, ANDREW RAPPE — Relaxor ferroelectrics are of fundamental scientific interest and are also used in a variety of applications, such as piezoelectric transducers and capacitors. They exhibit permittivity peaks that are broad with respect to both temperature and frequency. We have developed a bond-valence model for $Pb(Mg_{1/4}Ti_{1/4}Nb_{1/2})O_3$ (PMN-PT) and performed atomistic bond-valence molecular dynamics (BVMD) simulations of PMN-PT. We have studied relaxor behavior at a range of temperatures, in order to analyze polar nanoregion dynamics and relaxation lifetimes. We find that even for a fairly small simulation size of $6\times6\times6$ supercell (1080 atoms), the system exhibits frequency dispersion. We present the results of $6 \times 6 \times 6$, $8 \times 8 \times 8$ and $10 \times 10 \times 10$ supercell BVMD simulations, analyze the pair distribution function of the PMN-PT and elucidate the local chemical origin of relaxor behavior.

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