Molecular dynamics computational studies of relaxor ferroelectric behavior in Pb(Mg\textsubscript{1/4}Ti\textsubscript{1/4}Nb\textsubscript{1/2})O\textsubscript{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\textsubscript{1/4}Ti\textsubscript{1/4}Nb\textsubscript{1/2})O\textsubscript{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 6×6×6 supercell (1080 atoms), the system exhibits frequency dispersion. We present the results of 6×6×6, 8×8×8 and 10×10×10 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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