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Structure and dynamics analyses of $Pb(Mg_{1/3},Nb_{2/3})O_3$-$PbTiO_3$[1]
HIROYUKI TAKENAKA, DIOMEDES SALDANA-GRECO, ILYA GRINBERG, ANDREW M. RAPPE, University of Pennsylvania — Relaxor ferroelectric materials are of importance in applications due to their giant piezoelectricity, anomalous dielectric response, and diffuse phase transitions. However, mechanisms of the anomalous physical properties are still ambiguous, especially local structure and dynamics. According to our recent molecular dynamics simulations using a rock salt random site B-cation arrangement, the relax local structure is analogous to the hydrogen bonded network in water. In this work, we present structure and dynamics obtained from Bond-Valence model atomistic molecular dynamics simulations with the random site model and fully disordered 0.75PMN-0.25PT using diffuse scattering and dynamic pair distribution function techniques and compare our results with the available experimental data.

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