

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Molecular Dynamics Study of Dielectric Response in a Relaxor Ferroelectric ANDREW RAPPE, ILYA GRINBERG, University of Pennsylvania, YOUNG-HAN SHIN, University of Ulsan — We use atomistic molecular dynamics simulations to study relaxor behavior in the $0.75\text{Pb}(\text{Mg},\text{Nb})\text{O}_3\text{-}0.25\text{PbTiO}_3$ material. Even for a fairly small simulation size of 1000 atoms, the system exhibits frequency dispersion and deviation from the Curie-Weiss law typical of relaxor materials. Analysis of the time autocorrelation functions for individual atoms allows us to identify the Nb atoms with a high concentration of neighboring Ti atoms as the nucleation sites for the relaxor behavior. This is due to the higher coupling between the cation displacements induced by the presence of overbonded oxygen atoms located between Nb and Ti atoms.

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Date submitted: 08 Nov 2009

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