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### **Computational Study of Local Structure and Dynamics in a Relaxor Ferroelectric<sup>1</sup>**

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Relaxor ferroelectrics exhibit a stronger piezoelectric effect, diffuse phase transitions with high permittivity, and unique dielectric response with strong frequency dispersion which are exploited for technological applications and give rise to scientific interest. The diffuse phase transitions have been explained by widely accepted model of polar nanoregions inside a non-polar matrix. Recent experimental and theoretical results, however, suggest requirements of alternate interpretations of the origin of the relaxor behavior. Macroscopic elucidations of structure and dynamics in relaxors are still one of challenging topics in solid-state physics. We analyzed local structure and dynamics with dynamic pair distribution function and diffuse scattering techniques for  $0.75\text{PbMg}_{1/3}\text{Nb}_{2/3}\text{O}_3$ - $0.25\text{PbTiO}_3$ , a prototypical relaxor, performing molecular dynamics simulations. Our analysis showed phase transition temperatures in good agreement with experimental values. From inspections of in-phase motion correlations for Pb pairs, we found analogy between the phase transition from the paraelectric phase to the relaxor phase in the relaxor and the behavior of the couplings from high temperature to room temperature in water. We, therefore, propose alternate model.

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