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Origin of diffuse scattering in relaxor ferroelectrics

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High-pressure and variable temperature single crystal synchrotron X-ray measurements combined with first-principles based molecular dynamics simulations study diffuse scattering in the relaxor ferroelectric system PSN (PbSc1/2Nb1/2O3). Constant temperature experiments show pressure induced transition to the relaxor phase at different temperatures characterized by butterfly and rod shaped diffuse scattering around the {h00} and {hh0} Bragg spots, respectively. The simulations [1] reproduce the observed diffuse scattering features as well as their pressure-temperature behavior, and show that they arise from polarization correlations between chemically-ordered regions, which in previous simulations were shown to behave as polar nanoregions. Simulations also exhibit radial diffuse scattering (elongated towards and away from Q=(000)), that persists even in the paraelectric phase, consistent with previous neutron experiments on (PbMg1/3Nb2/3O3) (PMN). DFPT calculations to elucidate origin of Raman peaks in the relaxor phase will also be presented.

[1] P. Ganesh, E. Cockayne, M. Ahart, R. E. Cohen, B. Burton, Russell J. Hemley, Yang Ren, Wange Yang and Z.-G. Ye, Phys. Rev. B **81**, 144102 (2010)