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Effective Hamiltonian study of $PbSc_{1/2}Nb_{1/2}O_3$ under pressure ERIC COCKAYNE, SILVIA TINTE, BENJAMIN P. BURTON, NIST, UMESH V. WAGHMARE, JNCASR — In general, increasing pressure depresses the transition temperature T_{FE} of ferroelectric transitions, and sufficient pressure yields a FE $\rightarrow$ paraelectric (PE) transition. A more complicated behavior is observed for disordered $PbSc_{1/2}Nb_{1/2}O_3$ (PSN). At atmospheric pressure, PSN exhibits relaxor ferroelectric (RFE) properties within a small temperature range before transforming to a FE phase at low temperatures. Pressure of approximately 1.5 to 2.5 GPa induces a low-temperature RFE state without a RFE/FE phase boundary.[E. L. Venturini et al.] To investigate the effects of pressure on phase transitions in PSN, we used a first-principles based effective Hamiltonian. Our effective Hamiltonian includes a local field term arising from the charge difference between the Sc^{3+} and Nb^{5+} ions. Under pressure, the local field term changes little, while the FE well depths decrease, increasing the relative importance of the local fields. Molecular dynamics simulations show that T_{FE} decreases with temperature and that the phase transition broadens.

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