Thermal and quenched disorder in ferroelectrics

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Developments in machine learning and deep neural network representations make possible to study the ferroelectric phase transition, beyond mean field and reduced models, with molecular dynamics (MD) simulations of ab-initio quality. I will illustrate the approach with recent studies of two perovskite materials at ambient pressure: lead titanate (PTO), a prototypical ferroelectric crystal, and lead magnesium niobate (PMN), a chemically disordered perovskite that exhibits glassy behavior, called relaxor, and bears similarities with spin and fragile structural glasses. In both cases, simulations predict thermodynamic and dielectric properties in good agreement with experiment and provide fresh insight into the microscopic mechanisms of the transition. In PTO, a unified picture emerges that reconciles diffraction and optical experiments. In PMN, the simulations reveal quasi-localized vibrational modes that underlie universal glassy features.

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