Understanding Ferroelectrics with Universal Force Fields

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The functional performance of ferroelectric materials often relies on the interactions between polarization and external stimuli, which are intimately related to the dynamic responses of domains and domain walls. Molecular Dynamics (MD) is an ideal computational tool for investigating dynamic processes on large length and time scales while providing atomistic details with femtosecond time resolution. In this talk, I will discuss the development of universal force fields applicable to two important ferroelectric systems: hafnia and perovskite. Enabled by deep-learning-assisted MD simulations, we are able to understand new ferroelectrics like hafnia as well as uncover new physics in classic systems such as PbTiO□. Notable examples include ultrahigh oxygen ion mobility promoted by bias-driven successive ferroelectric transitions in HfO□ and a novel topological structure, the dipole spiral, in PbTiO□.