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### **Multiscale Simulations of Dynamics of Ferroelectric Domains<sup>1</sup>**

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Ferroelectrics with switchable polarization have many important technological applications, which heavily rely on the interactions between the polarization and external perturbations. Understanding the dynamical response of ferroelectric materials is crucial for the discovery and development of new design principles and engineering strategies for optimized and breakthrough applications of ferroelectrics. We developed a multiscale computational approach that combines methods at different length and time scales to elucidate the connection between local structures, domain dynamics, and macroscopic finite-temperature properties of ferroelectrics. We started from first-principles calculations of ferroelectrics to build a model interatomic potential, enabling large-scale molecular dynamics (MD) simulations. The atomistic insights of nucleation and growth at the domain wall obtained from MD were then incorporated into a continuum model within the framework of Landau-Ginzburg-Devonshire theory. This progressive theoretical framework allows for the first time an efficient and accurate estimation of macroscopic properties such as the coercive field for a broad range of ferroelectrics from first-principles. <sup>2</sup>This multiscale approach has also been applied to explore the effect of dipolar defects on ferroelectric switching and to understand the origin of giant electro-strain coupling.

<sup>1</sup>ONR, NSF, Carnegie Institution for Science

<sup>2</sup>S. Liu, I. Grinberg, and A. M. Rappe, *Nature*, 534, 360-363 (2016)