

## Computational Understanding and Prediction of Polar States in Ferroelectric Heterostructures Using Phase-field Method

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## Abstract:

This presentation will discuss the applications of the phase-field method to understanding and discovering new mesoscale polar states that might emerge from nanoscale ferroelectric heterostructures subject to different mechanical and electric boundary conditions. As an example, the determination of thermodynamic conditions and geometric length scales leading to the formation of ordered polar vortex lattice as well as mixed states of regular domains and vortices in ferroelectric superlattices of PbTiO<sub>3</sub>/SrTiO<sub>3</sub> using phase-field simulations and analytical theory will be presented. Switching of these vortex lattice states might produce other transient polar states such as polar skyrmions. It is shown that the stability of these vortex lattices involves an intimate competition between long-range electrostatic, long-range elastic, and short-range polarization gradient-related interactions leading to both an upper- and a lower-bound to the length scale at which these states can be observed. We further predicted the periodicity phase diagrams that show excellent agreements with experimental observations by collaborators.

## Monday, March 18, 2019 at 3:00 pm SERC, Room 116 Refreshments will be served at 2:45 pm