Abstract Submitted
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First-principles-based Landau energy functionals for perovskite ferroelectrics[1] KRISHNA CHAITANYA PITIKE, NEHA GADIGI, JOHN MANGERI, University of Connecticut, Storrs, VALENTINO COOPER, Oak Ridge National Laboratory, Oak Ridge, SERGE NAKHMANSON, University of Connecticut, Storrs — ABO_3 perovskite-oxide ferroelectrics are well known for their useful functional properties. These materials, as well as their solid solutions, exhibit rich phase diagrams that can be exploited, e.g., to obtain large piezoelectric and dielectric responses. Mesoscale-level investigations of their behavior usually utilize Landau phenomenological theory, where the system energy functional is represented by a polynomial expansion in powers of polarization and strain that is parameterized from experimental data. In this project, we present an approach for fitting the Landau functionals for perovskite ferroelectrics directly from first principles simulations with the help of statistical and machine learning tools. Initial data sets are created by computing the energies for a wide range of possible structural configurations involving polar and elastic distortions with standard density-functional theory (DFT) codes. A small fraction of this data is then processed by supervised machine learning algorithms to train a Landau-style polynomial model that can predict the system energies to within 20 meV of the DFT results.

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