Abstract Submitted
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Finite temperature properties of (Ba,Sr)TiO_3 disordered alloys and $BaTiO_3$/$SrTiO_3$ superlattices from first-principles[1] SERGEY LISENKOV, LAURA WALIZER, LAURENT BELLAICHE, University of Arkansas — We develop and use a first-principles-based scheme to predict properties of (Ba,Sr)TiO_3-based systems at finite temperature. This scheme yields a composition-versus-temperature phase diagram of disordered $(Ba_{1-x}Sr_x r)TiO_3$ solid solutions that is in rather good agreement with experimental data. We further use this scheme to reveal and understand the strain-versus-temperature phase diagram of several $BaTiO_3$/$SrTiO_3$ superlattices. A wide variety of dipole patterns, including homogeneous ferroelectric phase and periodic stripe patterns, are predicted to occur depending on the interplay between temperature, strain and superlattice periods.

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