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Temperature-dependent phase transition of ferroelectric perovskites: A Wang-Landau-DFT approach[1] SIMUCK YUK, YING WAI LI, MARKUS EISENBACH, VALENTINO COOPER, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — Since the discovery of ferroelectricity in perovskite oxides, considerable efforts have been devoted to understanding their phase transition behaviors in terms of temperature, pressure, and composition. Such materials have regularly been used in transducer and actuator applications. As our first step to make accurate predictions of the crystal phases of more complex oxides such as $Pb(Zr_xTi_{1-x})O_3$, we have used the Wang-Landau (WL) algorithm and density functional theory (DFT) to examine the temperature-dependent phase transition of $PbTiO_3$, $BaTiO_3$, and $KNbO_3$. DFT was employed to evaluate the energetics of important crystal-structure candidates, which were later used as the input for WL algorithm. In addition, we examine how the choice of exchange-correlation functionals affects our predictions of the relevant phase transition temperatures.

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