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Application of the Wang-Landau Algorithm applied to Ferroelectrics SAAD BINOMRAN, King Saud Univ, IGOR KORNEV, Laboratoire SPMS, UMR 8580 du CNRS, Ecole Centrale Paris, 92295 Chatenay-Malabry, France, LAURENT BELLAICHE, Institute for Nanoscience and Engineering and Physics Department, University of Arkansas, Fayetteville, Arkansas 72701, USA —
The conventional description of phase transitions in ferroelectrics is based on canonical thermodynamic functions and always assumes the thermodynamic limit of an infinite system. However, ferroelectrics at nanoscale recently became of high interest due to their potential applications in minuaturized devices. It is this timely and more appropriate to use the microcanonical ensemble when mimicking ferroelectric systems. Here, a first-principles-derived scheme, combined with an efficient Monte Carlo microcanonial technique, is used to gain new insight into the paraelectric to ferroelectric phase transition and the effect of the electric field on properties of $BaTiO_3$ systems. In this presentation, we will show the temperature variation of the specific heat for different lattice sizes in $BaTiO_3$ systems. The nature of the phase transition and the behaviour of the specific heat versus the lattice size will be documented. In addition, the effect of the electric field on the character of the phase transitions in BaTiO3 systems will be investigated by showing the free energy (F) versus the internal energy (U) curves. Electrocaloric effects can also be easily computed and will be discussed.

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