Application of the Wang-Landau Algorithm applied to Ferroelectrics

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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 [1,2].

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. More precisely, we use a Wang-Landau algorithm [3]**,** which is an efficient and accurate method for the study of the phase transitions. Since such algorithm computes the density of states, g(E), one can then calculate most thermodynamical quantities for all temperature with one single simulation! Moreover, the free energy (F) and the entropy (S) can be readily calculated, unlike in conventional Monte Carlo Metropolis simulations – which allows the investigation of challenging but important quantities.

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.
We are confident that our results lead to a deeper understanding of phase transitions in ferroelectrics, in general, and may help in interpreting future experimental data, in particular.

We also hope that it can have an impact in designing new and improved devices for actuators, sensors, optical switches, RF devices and memory storage.

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References:

[1] D. Gross, Microcanonical Thermodynamics: Phase Transitions in "small" Systems, World Scientific lecture notes in physics (World Scientific, 2001), ISBN 9789812798916.

[2] M. Pleimling and H. Behringer, Phase Transitions 78, 787 (2005).

[3] F. Wang and D. P. Landau, Phys. Rev. Lett. 86, 2050 (2001).