Simulating domain structure in perovskites using machine learning and molecular dynamics

Summary

The accurate description of the structural and thermodynamic properties of ferroelectrics has been one of the most remarkable achievements of Density Functional Theory (DFT). However, running large simulation cells with DFT is computationally demanding, while simulations of small cells are often plagued with non-physical effects that are a consequence of the system's finite size. Recently, we demonstrated that one can train a machine learning on the energies and forces from DFT and then use the learned potential to simulate large simulation cells [1]. This technology allowed us to systematically investigate these finite size effects by performing simulations over long time and length scales. The objective of this PhD is to extend this work by using machine learning models that include an explicit description of electrostatics. The resulting model will then be used to calculate the energy of a domain wall.

Project

A ferroelectric is a material that possesses a permanent electric polarisation that can be switched under the action of an external electric field Typically, the emergence of the polar phase is accompanied by a structural transition from a high-symmetry paraelectric state down to a broken-symmetry state with a characteristic long-range dipolar ordering. This effect is of wide use in technological applications, for instance in capacitors, where ferroelectrics are used as a high-k dielectric medium for effective energy and charge storage, as well as in piezoelectric devices, sensors and field-effect transistors.

Density functional theory (DFT) calculations have completed experimental efforts that have sought to understand the microscopic structure of ferroelectrics. Typically DFT has been used to study these types of systems over small length and time scales because this method is computationally expensive. Meanwhile, less-accurate, empirical models have been used to long length and time scale phenomena in such systems. The development of machine learning techniques ensures that these empirical models are no longer necessary as we can now use DFT calculation to train a relatively inexpensive model that can be used to perform simulations over long length and time scales with DFT accuracy.

Our earlier work [1], has demonstrated that you can use machine learning potentials to simulate the phase transitions that occur in these ferroelectric materials. However, thus far the modes that we have trained have had no explicit description of the electrostatic interactions that make these materials so interesting. In this project you would thus first fit a machine learning that includes an explicit description of the electrostatic interaction. Once this was done we would then use the model that you have developed to study the domain wall energy using techniques like those discussed in these papers [2,3,4].

Bibliography

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