Understanding thermal transport in ferroelectric materials using molecular dynamics and machine learning

Ferroelectric materials exhibit spontaneous electric polarization that can be switched by an applied electric field. At present, they are commonly used in piezoelectric sensors, actuators and high-k capacitors, but their switchable polarisation and associated domain structure makes them promising candidates for a variety of next generation applications, such as memories and nanoelectronic devices. One aspect that attracted growing interest is using ferroelectric materials for thermal management applications. The ability to reconfigure ferroelectric domain microstructure with an electric field provides a means to tune the phonon scattering rates and therefore create a thermal conductivity switch. As well as this, some ferroelectrics can actively self-cool through the 'electrocaloric effect', Here, a rapid cooling of the material bulk is triggered by electric field induced changes in dipolar entropy, which can also be affected by ferroelectric microstructure.

However, the thermal transport properties of ferroelectric materials are still not well understood. This is due in part to the complex microstructure of these materials, which can have a significant impact on their thermal conductivity. In this PhD project, you will use molecular dynamics simulations to investigate the thermal transport properties of ferroelectric materials.

In the project you will learn to use state of the art machine learning methods to train a model that describes the interactions between the atoms. When training this model, you will need to determine accurate energies of structures using calculations that are based on quantum mechanics.

There has been longstanding interest in performing experiments on ferroelectric materials within the physics department at Queen's University Belfast. However, the theoretical and modelling groups in the department have not performed many studies on these materials. This PhD project is in part an effort to create more synergy between the work being done in the labs and the work being done with computer simulation. You will thus have many opportunities to interact with experimental colleagues. You will also be at the forefront as we build a new and important research activity within the school.

Supervisory team

Gareth Tribello (g.tribello@qub.ac.uk) (primary supervisor), David Wilkins (d.wilkins@qub.ac.uk) (secondary supervisor) and Raymond McQuaid (r.mcquaid@qub.ac.uk) (secondary supervisor)

Entry requirements

Applicants are expected to possess a first or upper-second class degree in physics, chemistry, mathematics, or a relevant discipline (or an equivalent overseas qualification), or a lower second-class degree along with a Master's degree.

How to apply

Applications should be submitted via the Direct Applications Portal.

References

1. L. Gigli *et al.* **Thermodynamics and dielectric response of $BaTiO_3$ by data-driven modeling** NPJ Computational Materials 8, 1-17 (2022)
2. L. Gigli *et al.* **Modelling the ferroelectric phase transition in barium titanate with DFT accuracy and converged sampling** arXiv :2310.12579 (2023)
3. S. Li *et al.* **Strain-controlled thermal conductivity in ferroic twinned films** Scientific Reports, 4 6375 (2014)
4. A. Negi *et al.* **Thickness-dependent thermal conductivity and phonon mean free path distribution in single-crystalline barium titanate** Advanced Science 10, 2301273 (2023)
5. J. Iniguez and R. Rurali **A phononic switch based on ferroelectric domain walls** Physical Review B, 96, 140101 (2017)
6. J. A Seijas-Bellido **Anisotropy-driven thermal conductivity switching and thermal hysteresis in a ferroelectric** Advanced Physics Letters 115, 192903 (2019)