PhD Position

Molecular dynamics simulations of the influence of ferroelectric topological structures on thermal conductivity

Fascinated by exploring the frontiers of materials science and uncovering new physics? Join our team! We are seeking a PhD student to simulate and investigate the fundamental properties of complex ferroelectric structures.

Context

Since the early days of computing, hardware has evolved from mechanical to digital systems, where logic operations are performed by controlling electrons in semiconductors. However, the development of semiconductor-based chips is encountering important bottlenecks. To be disruptive, future progress is expected to be driven by different information carriers or different computing paradigms. For these alternatives, oxides, and in particular ferroelectrics, already show great promise and are the ideal solid-state materials for **a new type of computing based on thermal currents rather than electric currents** [1].

Ferroelectric materials spontaneously exhibit regions of uniform electric polarization, called domains. They are separated by topological defects known as domain walls [2]. The number of domains and their orientations can be controlled by applying an electric field (Fig. 1). Experimentally, it has been shown that **domain walls can be used to tune the thermal conductivity in solid-state materials** [3]. In general, **the atomic structure of interfaces, and its related interfacial thermal resistance, controls the thermal conductivity in nanomaterials** [4] and is sometimes inducing emerging exotic properties, such as thermal rectification or ballistic heat transport [5].

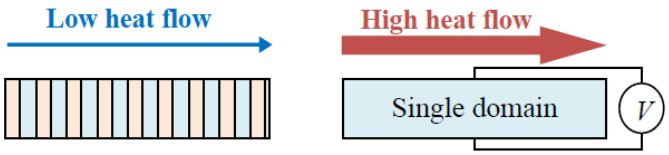

Figure 1. Schematic of the influence of domain walls on thermal conductivity.

Project description

For this PhD thesis, you will use **molecular dynamics simulations to investigate several parameters that could influence the thermal conductivity in ferroelectric materials, starting with perovskite materials such as $BaTiO_3$**. You will study the influence of the number of domain walls, the direction of the domain walls with respect to the heat flow, the influence of temperature and of the geometry of the system (**bulk**, **thin film**, **freestanding membrane, superlattice**). The topic is a continuation of a previous successful internship where preliminary calculations were performed.

[1] Nataf *et al.* Using Oxides to Compute with heat, Nature Rev. Mater. 9 (2024)
[2] Nataf *et al.* Domain-wall engineering and topological defects in ferroelectric and ferroelastic materials, Nature Rev. Phys. 2 (2020)
[3] Belrhiti-Nejjar, … Nataf. Domain-Wall Driven Suppression of Thermal Conductivity in a Ferroelectric Polycrystal, Advanced Science 06931 (2025).
[4] Merabia, Termentzidis, Thermal conductance at the interface between crystals using equilibrium and nonequilibrium molecular dynamics, Phys. Rev. B 86 (2012)
[5] Desmarchelier, Carré, Termentzidis, Tanguy. Ballistic heat transport in nanocomposite: The role of the shape and interconnection of nanoinclusions, Nanomaterials 11 (2021)

Location, salary, dates

The PhD student will be **working in the GREMAN laboratory (UMR CNRS 7347) in the University of Tours** (Parc Grandmont, 37200 Tours). You will be enrolled as PhD student at the doctoral training school of the University of Tours, where you can benefit from a tailored training programme to acquire transferable, discipline-related and research skills. The following video will introduce you the University of Tours. The GREMAN laboratory has strong expertise in both ferroelectric oxides and molecular dynamics simulations. You will also **have short stays in the CETHIL laboratory in Lyon**, where you will be co-supervised by Konstantinos Termentzidis, an expert on simulations of thermal transport in nanomaterials.

Experimental works on the influence of ferroelectric topological structures on thermal conductivity is already carried out in the GREMAN laboratory, as part of the ERC Starting Grant DYNAMHEAT and the ANR PRC SUPER. Within this context, **you will join a vibrant international** team. You will contribute to an interdisciplinary team of physicists, materials scientists, engineers and chemists. The environment is open and collaborative, promoting daily interaction and knowledge exchange. You will also interact with international collaborators (Jorge Íñiguez-González, LIST, Luxembourg; Yun Hee Jang, DGIST, Korea).
The starting date of the **3-years** PhD position is **1st October 2026**. It is a fixed term contract (36 months) with a gross monthly salary of ~2,300.00 €.

Candidate profile

The candidate should have a master's degree preferably in physics, chemistry or materials sciences. They must be motivated and dynamic with **strong abilities in theoretical work**. A good command of the English language is required, both written and oral (at least B2 level). Internship experience in a research laboratory will be appreciated. **Experience with simulations** and/or ferroelectric materials and/or thermal conductivity would be a plus.

How to apply

Prospective candidates should send their **detailed CV**, a **cover letter** and the contact details of **at least one reference** by email no later than **20/03/2026** to the three PhD supervisors:
Guillaume Nataf (GREMAN): guillaume.nataf@univ-tours.fr
Yves Lansac (GREMAN): yves.lansac@univ-tours.fr
Konstantinos Termentzidis (CETHIL): konstantinos.termentzidis@insa-lyon.fr

The most promising candidates will be invited for an interview.