A Grenoble, au centre des Alpes, le CEA-Leti est un institut de recherche appliquée en micro et nano technologies, technologies de l'information et de la santé.
Interface privilégiée du monde industriel et de la recherche académique, il assure chaque année le développement et le transfert de technologies innovantes dans des secteurs variés via des programmes de recherche utilisant nos plateformes technologiques.

Research areas: computational physics, machine learning, nanotechnologies

Thermal transport in van der Waals superlattices by equivariant deep learning models

Among the next generation nonvolatile memories (NVM), Phase Change Memory (PCM) technologies based on chalcogenide materials, such as GeSbTe (GST), are the most mature. Thermally driven phase transitions of the phase change material are achieved using electrical pulses in order to switch between a low resistive crystalline state and a high resistive amorphous state.

Recently, chalcogenide superlattices (SL) formed by the alternate stacking of ultrathin layers separated by van der Waals (vdW)-like interfaces (e.g. $GeTe/Sb_2Te_3$ or $GeSb_2Te_4/Sb_2Te_3$) have been reported to improve the energy efficiency of PCMs. SL interfaces are expected to play a key role in the electrical performances of these devices.

Simulations using molecular dynamics (MD) are particularly suitable to study the physical properties of these materials at the atomic scale but require an accurate description of the potential energy surface (PES). In the past couple of years, much progress has been made in the development of machine learning interatomic potentials (ML-IP) to describe complex systems. Recently, ML-IP relying on E(3)-equivariant deep learning models have shown very high accuracy and data efficiency compared to other ML-IP methods.

The goal of this internship is to employ MD simulations to study the heat conduction mediated by lattice vibrations in chalcogenide SL materials using the Green-Kubo formalism and E(3)-equivariant ML-IPs. The candidate will first have to train a potential to study GST materials using a dataset of reference systems obtained from density functional theory (DFT) calculations. Then, the thermal transport in chalcogenide SLs will be studied using MD simulations with the LAMMPS code (https://lammps.sandia.gov/). The simulations will be carried out on high-performance computing (HPC) resources with GPU accelerators.

Required skills:

- Background in solid state physics and chemistry or related fields
- Programming using Python and C++
- Understanding of Linux and parallel computing is desirable
- Previous experience with machine learning techniques is a plus

Position location: Grenoble, France
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Prepared diploma: Bac+5 – Master 2
Duration: 6 months
Position start date: Feb. 2023
PhD opportunity: Yes