A Grenoble, au centre des Alpes, le 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.

Domaine de recherche: computational physics, machine learning, nanotechnologies

Intitulé du stage : Deep learning for large scale molecular dynamics simulation of chalcogenide materials

Cadre et contexte

Among next generation nonvolatile memories (NVM), Phase Change memory (PCM) is the most mature one. CEA Leti is currently working on the development of this technology in collaboration with industrial partners. However several technological issues require a fine understanding of the underlying physical mechanisms at the atomic scale. Simulations using large scale molecular dynamics (MD) are particularly suitable to investigate these phenomena but require accurate interatomic potentials to describe the potential energy surface (PES). In the past decade, much progress has been made in the development of interatomic potentials using machine learning techniques to describe complex systems.

Travail demandé

The goal of this internship is to set up a Neural Network potential (NNP) based on the Behler-Parrinello method (Phys. Rev. Lett. **98**, 146401 (2007)) using large scale MD. The candidate will first have to realize a literature review on neural networks and their application to solid state problems. Then, she/he will implement a NN algorithm using deep learning libraries such as TensorFlow. The NNP will finally be trained with a large database of reference systems obtained from DFT calculations for a binary chalcogenide material. The NNP will be also implemented in the LAMMPS code (https://lammps.sandia.gov/) to perform MD simulations. A special attention will be given to the validation of the NNP.

Required skills:

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

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Formation Requise: Master 2
Durée: 6 months
Date démarrage: Feb. 2019
Possibilité de thèse (oui/non) oui