Thermal and phase transition properties of van der Waals heterostructures by equivariant graph neural networks

Description:

The recent progress in the synthesis of 2D materials, such as transition-metal dichalcogenides (TMD) and van der Waals (vdW) heterostructures, shows a promising path for next-generation electronics that are currently being developed at CEA-Leti. In particular, control of phase transitions in such systems finds many technological applications such as nonvolatile memories (NVM) or radio-frequency (RF) switches. Understanding of the thermodynamics and the kinetics of 2D phase transitions is fundamental for the development of these devices. Theoretical calculations are essential to study phase transitions. Simulations using molecular dynamics (MD) are particularly suitable to study the physical properties of complex materials at the atomic scale, but require an accurate description of their potential energy surface (PES). In the past couple of years, much progress has been made in the development of machine learning interatomic potentials (MLIP) trained on *ab initio* simulations to describe such PES. Recently, MLIP relying on equivariant graph neural networks (GNN) have shown very high accuracy and data efficiency compared to other MLIP methods.

The goal of this PhD is to study phase transition properties in 2D materials and vdW heterostructures by means of MD simulations with equivariant GNN interatomic potentials. The successful candidate will also investigate thermal properties and electric field-driven phase transitions. This PhD thesis will be an opportunity to develop new computational methods based on deep learning technique for simulations of materials at the atomic scale.

Candidate profile:

We are looking for highly motivated candidates with a master's degree in condensed matter physics or chemistry and a strong interest in computer science and machine learning. The candidate should have some experience in python and/or C++ programming , as well as a solid background in condensed matter physics. Applications should include a brief cover letter, a CV, a transcript of the master's degree and contact information for at least two references, to be sent to the supervisors:

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