O.19 Accelerating the computation of finite-temperature properties with Machine-Learning Assisted Canonical Sampling

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Ab Initio Molecular Dynamics (AIMD) is a powerful method which allows to sample the canonical ensemble in order to study the effects of finite-temperature. Unfortunately, due to its high computational cost, AIMD is usually reserved to the simplest systems. On the other hand, recent progress in Machine-Learning based Interatomic Potential (MLIP) has the potential to greatly accelerate the study of finite-temperature properties. However, the training of a MLIP is a tedious task, requiring a careful selection of atomic configurations, which are often obtained using AIMD.

In this talk, we will present the Machine-Learning Assisted Canonical Sampling (MLACS) method. Being based on a variational principle, MLACS uses a self-consistently constructed MLIP to create atomic configurations that best approximate the canonical ensemble of the DFT potential, in a fraction of the cost of AIMD. As a result, a reduction as high as two order of magnitude in human time and one order of magnitude in CPU time is accessible, all while keeping a near-DFT accuracy.

We will present our implementation of the method, which is build on the link of the Abinit Software with the SNAP potential in LAMMPS[1] and the Atomic Simulation Environnement (ASE)[2].

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[1] Thompson *et al*, J. Comp. Phys. **285**, 316 (2015).

[2] Larsen *et al*, J.Phys. Condens. Matter **29**, 273002 (2017).