Seminar

Gaussian Approximation Potentials - and an Alternative Solution - for Molecular Dynamics

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Abstract

To theoretically study material properties, frequent molecular dynamics (MD) simulations are conducted, in which the evolution of the atomic system is governed by the classical equations of motion under a general interatomic potential. Even though MD is a widely used technique in academia and industry, researchers employing it face a long-standing dilemma: accuracy vs. efficiency. On the one hand, *ab initio* methods, such as density functional theory (DFT), offer high accuracy; however, their prohibitively high computational costs limit their application to only relatively small systems ($<10^3$ atoms) and short simulation times ($\sim 10^1$ ps). On the other hand, empirical potentials, which are simpler mathematical expressions parametrized to reproduce experimental results, require much less computational resources; however, their accuracy is not sufficient for many applications. Moreover, they are, in general terms, only suited for the specific application for which they were developed, therefore severely limiting their generalizability.
In this context, machine learning (ML) interatomic potentials gained a lot of interest in recent years, due to their attractive cost-to-accuracy ratio, as they are very often able to combine *ab initio* level accuracy with computational times similar to those of empirical potentials. These interatomic potentials work by training a ML model to act as a computationally efficient surrogate model of the potential energy surface (PES).
In this seminar, we present the results of recently developed ML interatomic potentials at Technische Universität (TU) Wien for modelling amorphous silicon nitride (Si_3N_4), simulating neutron irradiation in SiGe and studying the oxidation process of Si. Our developments are based on the Gaussian approximation potential (GAP) method, an efficient ML algorithm which works by comparing the input atomic environment to those available in its training dataset. Moreover, an alternative solution to ML interatomic potentials will be presented, as well as future work on developing a neuromorphic hardware accelerator for ML-based MD.