**Advancing interatomic potentials for molecular dynamics simulations of 2D materials**

**Idea:** The idea of this master thesis is to compare the different interatomic potentials in terms of accuracy and efficiency. For example, the candidate can compare machine learning potentials (GAP for example which is the most promising) with usual classical potentials (Tersoff, AIREBO, ILP, etc.), and also benchmark these results against DFT and experimental results. The thesis can be centered around 2D materials of current interest for example: graphene, hBN, TMDs. By accuracy one means the lattice constants, elastic constants, phonon bands, DOS, and by efficiency one means the speed of the calculations when comparing the different results (this would not involve the DFT part, just the MLIP implementation in LAMMPS), and convenient parallelization.

**Bibliography:**


- J. Phys. Chem. A 2020, 124, 731−745
- J. Phys. Chem. C 2020, 124, 22278−22290
- Tersoff, J. Modeling solid-state chemistry: Interatomic potentials for multicomponent systems. Phys. Rev. B: Condens. Matter Mater. Phys. 1989, 39, 5566−5568.
- Bartók, A. P.; Payne, M. C.; Kondor, R.; Csá nyi, G. Gaussian Approximation Potentials: The Accuracy of Quantum Mechanics, without the Electrons. Phys. Rev. Lett. 2010, 104, 136403.
- van Duin, A. C. T.; Dasgupta, S.; Lorant, F.; Goddard, W. A., III ReaxFF: A Reactive Force Field for Hydrocarbons. J. Phys. Chem. A 2001, 105, 9396−9409.


**Catch:** Molecular dynamics is the initial step into gaining insight about the properties of materials in the nanoscale regime. For these simulations to be accurate we need an accurate representation of the potential energy surface (PES), in particular one with a good description of the phonon dispersion spectrum, which determines various mechanical and thermodynamical properties. Quantum mechanical approaches such as DFT or AIMD based on DFT offers good descriptions, but they represent a high computational cost and poor scaling (in the order of the cube of the electron number), this limits the number of atoms and the simulation time. Interatomic potentials (IAPs) appear as an alternative. IAPs are empirical parametrization of the PES based on functional forms that depend on the atomic degrees of freedom. In recent years, the rise of machine learning has provided an alternative to the development of IAPs with an accuracy close to ab initio methods, but with a much lower computational cost. Machine learning interatomic potentials (ML-IAPs) describe the PES as a function of local atomic environment descriptors, thus achieving invariance in rotation, translation, and permutation of atoms. Despite the fact that ML-IAPs have proven to be a good alternative there is still a lot to do in terms of describing strengths and weaknesses when using them in different scenarios.