Modelling mechanical properties of 2d materials

In this project, we will investigate the mechanisms of solid lubrication using Molecular-Dynamics simulations. In lubrication with a solid powder, small, nm-thin flakes of the solid slide easily past eachother. While we have some understanding of the behaviour of single sliding flakes, we are only beginning to explore the effects of having multiple flakes that can act collectively, or how multiple layers interact with each other [1].

This project will focus on possible effects of tearing of layers, as well as the interactions between layers. Another possible line of inquiry is the interactions between flakes. You will employ the existing openly available molecular dynamics code LAMMPS in combination with python scripting to create the models and to analyze the results.

[1] *Understanding the friction of atomically thin layered materials*, David Andersson and Astrid S. de Wijn, Nature Communications **11**, 420 (2020).

Recommended background

A basic programming course and an interest in modelling or programming. Tribology, basic statistical mechanics, or classical mechanics.

Supervisor

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Research environment: `http://syonax.net/science/research.html`.

Resources

The project will make use of high-performance computing resources that are already available through NTNU IT's HPC facilities and Sigma2.

Work load

This project is intended for a combined specialization project thesis and master thesis, i.e. 45 or 60 ECTS in total.

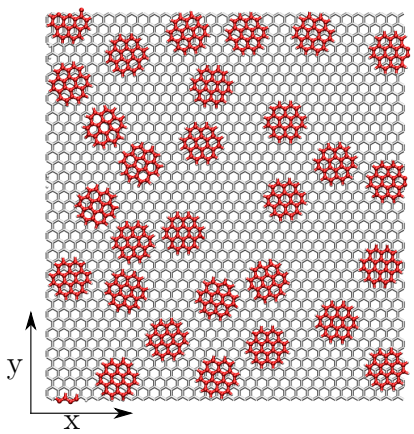

Figure 2: A top view of a simulation of a single layer of graphene flakes acting as a solid lubricant.