Lab 2 – Molecular dynamics

Goal: Learning the software *Lammps* and *Phonopy*, including visualization with VMD and matplotlib.

Activities: Let's follow the tutor who will explain *Lammps* input and output on the following problems:

- Lennard-Jones (LJ) coupled particles (basics from https://lammpstutorials.github.io/sphinx/build/html/tutorials/level1/lennard-jones-fluid.html)
- Water fluid (parts obtained from https://lammpstutorials.github.io/sphinx/build/html/tutorials/level2/polymer-in-water.html)
- Ethane molecule
- Graphene sheet (parts from https://lammpstutorials.github.io/sphinx/build/html/tutorials/level1/breaking-a-carbon-nanotube.html)

Lammps documentation is available at https://docs.lammps.org/Manual.html and we will actively use it.

We want to study lattice vibrations in solids based on Quantum Espresso and Phonopy and apply it to Cu.

Please note *that we provide only the notebooks. It is necessary that you execute the notebooks by yourself.*

Exercises at lab/home:

0. Make a review of the reports from Lab 1. Has the other group satisfyingly answered all questions? How does their solution compare to yours? Give constructive feedback on the report and post two critical questions about the results that the other group has. Grade the report with a 'U' or 'G'. This time, Group (i) reviews group (j)

Group (i)	Group (j)
1	2
2	3
3	4
4	5
5	6
6	1

1. In Lab 2, we introduced Lammps as a tool to perform molecular dynamics. Let's consider the introduction example about Lennard-Jones coupled particles and let's modify the provided input file accordingly to the following subtask:
    a. What happens when you skip the initial relaxation?
    b. What happens when step-wise increasing the temperature?
    c. What happens to the energies and intrinsic temperature when including more particles?
    d. What happens, when you increase the cut-off radius of the Lennard Jones potential?
    e. What happens when you use the Born-Mayer-Huggins potential instead of the LJ?

    Write a small summary about what happens when changing requested input and why it changes.

2. Go into the Lammps documentation or use a LLM to find out the meaning of the following input parameters
    a. pair_style born
    b. bond_style and bond_coeff
    c. angle_style and angle_coeff
    d. dihedral_style and dihedral_coeff
    e. improper_style and improper_coeff
    f. dump and dump_modify
    g. delete_atoms
    h. region and group

Write a small summary on each input parameter.

3. Use the example of the graphene sheet. Try to arrange a setup with two layers of graphene as well as length of 15nmx5nm and visualize the dynamics. Use otherwise the same setup we provided for the single sheet of graphene.
4. Use the Quantum Espresso input provided to you GaAs. Perform a calculation of phonon band structures as well as phonon density of states. Note, that GaAs might take a while to calculate.