Exercise 8 – Computational Materials Engineering

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Goals:

- Learn how to calculate energy barriers between local minima
- Learn how temperature helps to overcome energetic barriers
- Understand the concept of vacancy diffusion
- Understand the concept of a Berendsen thermostat
- Learn how to post-process simulation data

In this exercise sheet we want to examine vacancy diffusion in a crystal and its dependence on temperature.

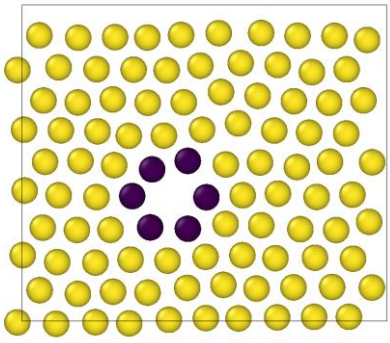
Tasks

Task 1: Download the files *A_equil_lattice.py*, *MorseCalculator.py* and *hexagonal_lattice.xyz* from ILIAS and save them in a newly created folder. For the sake of simplicity and to reduce the computational burden we investigate a two-dimensional hexagonal lattice of atoms. Open *hexagonal_lattice.xyz* with OVITO to visualize the system. How would you restrict the movement of the atoms to a single plane? As usual, we use the Morse potential for the interaction of the atoms. Open *MorseCalculator.py* to see an implementation of this constraint.

Task 2: Run *A_equil_lattice.py* to equilibrate the lattice at 600 K. Why do we need to initialize a non-zero velocity of the atoms? Why do we only set the velocity to a finite value in the lattice plane? If you do not know the answer, modify the script such that there is also a finite velocity in the direction perpendicular to the surface plane, run the script and investigate the trajectory.

Task 3: Download *B_diffuse_template.py*. The script deletes a single atom in order to create a vacancy in the lattice. Extend the script to also perform a subsequent NVE simulation with a timestep of 5 fs for 10000 steps. The simulation might take some time.

Task 4: Open the trajectory resulting from task 3 and observe the diffusion of the vacancy. If you were asked to plot the position of the vacancy as a function of time, how would you extract this information from the trajectory? Perform a *Coordination Analysis* in OVITO (can be found in the *Add modification* dropdown menu) using a cutoff radius of 3.6 Å. This analysis calculates the number of atoms within the chosen cutoff for each particle, the so-called coordination. Add the *Color coding* modification to color the atoms according to their coordination. The result should look like this:



The position of the vacancy can apparently be calculated from this information. Download *C_extract_movement.py*, run the script and understand how it calculates the position of the vacancy.

Task 5: Plot the different positions of the vacancy, the x-position on the x-axis and the y-position on the y-axis.

Task 6: Now we want to approximately calculate how much energy is needed to move the vacancy from one lattice site to a neighboring one. For this purpose we start from the relaxed lattice, create the vacancy and manually move one neighboring atom into the vacancy (such that the vacancy effectively wanders by one lattice site). Download, run and understand the script *D_barrier.py*. Calculate the energetic barrier (i.e. the maximal minus the minimal energy along the path). What is the configuration corresponding to the highest energy along the path?

Task 7: How does the diffusion process depend on the temperature? What do you expect? If you have time and motivation, redo tasks 2-5 with different initial temperatures and compare the results.