Computational Materials Science 2014
Exercises

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Crystal structures II
Total energy

1. **Lattice sums** (Analytical task)
   The lattice sum A_n^{crystal} shall be defined as

$$A_n^{\text{crystal}} = \sum_{\text{atom}\in\text{crystal}} \alpha_{\text{atom}}^{-n}, \tag{1}$$

   where the dimensionless quantity α_{atom} is the scaling factor of the distance of the atom to any freely chosen, but fixed reference atom and the nearest neighbor distance a_{Neighbor}:

$$\left|\vec{R}_{\text{atom}} - \vec{R}_{\text{ref}}\right| = \alpha_{\text{atom}} a_{\text{Neighbor}}. \tag{2}$$

   Compute the lattice sums A_6 and A_{12} up to the third nearest neighbor distance for the sc, bcc, and fcc lattice structure. Why are these quantities important to determine the total energy of noble gas lattices such as the Argon crystal?

2. **Melting an Argon crystal** (Tool task)
   In this task we determine the melting temperature of Argon, based on the modified Lennard-Jones potential introduced in the last exercise. This time we use *MiniMol* to perform a molecular dynamics simulation. The simulation is divided in two parts.

   a) Perform a temperature initialization MD run. Start with a fcc argon crystal structure (experimental lattice constant = 5.260 Å). Simulate an argon block with at least 500 atoms in a significantly larger simulation cell. This can be achieved e.g. with the *aims2minimol.py* tool, using the *cluster* option or by editing your MiniMol geometry file directly. Check that the system is equilibrated by plotting energies, temperature, and pressure over simulation steps. These quantities are listed in the MiniMol output. How many simulation steps are necessary to equilibrate the system?

   b) Run a micro canonical MD (NVE) starting from the equilibrated structure for at least the same time as the initialization run and visualize the resulting atomic structure. The geometry file provided by "MiniMol" can be directly visualized by *VESTA*, if the file suffix is renamed ".xyz".

   Perform this simulation for the temperatures $\theta \in \{20K, 60K, 100K\}$ and visualize the resulting atomic structures. In what kind of aggregate state is argon at these temperatures according to your atomic structures? Describe your criteria to distinguish between the aggregate states. To support your work, please hand in your control files and geometry files, together with screenshots of the resulting clusters. Note: We will do a more quantitative analysis of these simulations as part of the next homework. Stay tuned ... ;-)

⟶ Please, turn page.

Hint: The MiniMol control file for an NVT-MD initialization
Please note that comments in the control file are **not** supported!

```
Ar crystal melt          # Project name
MD                       # Calculation type MD = Molecular Dynamics
model_Ar_MLJ             # Model potential
geometry.minimol         # geometry file input
ar-temp-init.minimol     # geometry file output
100                      # print out data every N.th step
0                        # atomic density, if set to zero atomic density is not checked
1.25                     # a skin value to set up the neighbors list (1.25 is ok)
10000                    # maximum number of MD steps
0.001                    # size of time difference between steps in ps
***θ***                  # ***θ*** is temperature in K requested (if negative NVE is performed)
NH                       # thermostat type (NH = Nose-Hoover)
-1                       # control parameter for thermostat (negative = defaults)
256                      # integer seed for random number generator, allows for reproducible results
```

Hint: The MiniMol control file for an NVE-MD run
Please note that comments in the control file are **not** supported!

```
Ar crystal melt          # Project name
MD                       # Calculation type MD = Molecular Dynamics
model_Ar_MLJ             # Model potential
at-temp-init.minimol     # geometry file input
ar-result.xyz            # geometry file output
100                      # print out data every N.th step
0                        # atomic density, if set to zero atomic density is not checked
1.25                     # a skin value to set up the neighbors list (1.25 is ok)
10000                    # maximum number of MD steps
0.001                    # size of time difference between steps in ps
-1                       # temperature in K requested (if negative NVE is performed)
NH                       # thermostat type (NH = Nose-Hoover), is neglected since temperature is negative
-1                       # control parameter for thermostat (negative = defaults)
256                      # integer seed for random number generator, allows for reproducible results
```

Hint: The MiniMol geometry file
Please note that comments in the geometry file are **not** supported!

```
500                                        # Number of atoms
% N 2680.000000 2680.000000 2680.000000 # Lengths of simulation cell in Å '% N <xLen> <yLen> <zLen>'
Al 1005.000000 1005.000000 1005.000000  # Atom coordinates in Å <Symbol> <x> <y> <z>
Al 1007.680000 1007.680000 1005.000000
Al 1007.680000 1005.000000 1007.680000
Al 1005.000000 1007.680000 1007.680000
...                                        # and so on ...
```