1 Observing CIF crystal structures using ASE

A helpful tool to create and modify molecule or bulk structures is the Atomic Simulation Environment (ASE). We will use this software to create our own crystal structures and save them as CIF files.

1. Visit the ASE homepage: `https://wiki.fysik.dtu.dk/ase`
2. Look at available calculators listed on the start page
3. Scan the gallery for common use cases
4. Load your CIF file
5. Check the data structure via getter-functions as described in the ASE atoms object reference: `https://wiki.fysik.dtu.dk/ase/ase/atoms.html`

2 Build your own structure using ASE

1. Build a bulk structure with the same parameters (angles, atom positions, lattice constants) as given in your CIF file using ASE. You can follow this tutorial from the documentation: `https://wiki.fysik.dtu.dk/ase/ase/spacegroup/spacegroup.html`
2. Compare the resulting cell with the one that has been obtained by simply loading the CIF file into ASE.
3. Repeat the last task but this time use the `build` module provided by ASE to create the cell. `https://wiki.fysik.dtu.dk/ase/ase/build/build.html`

   What changes? Which one might take less computational time for a ground state calculation?
4. Write your cell as CIF file and have a look at the content. Do you recognize any peculiarities?

3 Fun fact - Have a guess!

How many HDDs (each able to hold 1 TB of data) are required in order to store the ground state of a H_2O molecule with 10 values per electronic coordinate for a single time step?

Hint 1: The H_2O molecule contains 2x1(H) + 1x8(O) = 10 electrons
Hint 2: The unapproximated many-body state is a function of all 10x3 = 30 coordinates