## 1 Linux introduction

Linux is *the* main tool for scientific computation. Virtually all important scientific software is available for the Linux OS, usually in form of plain source code, so it can be compiled for your specific hardware in order to run highly optimized. This is a crucial point since physical or chemical computations can easily take several days to weeks or even months. It is therefore necessary that users of such computer programs are familiar with the basic commands on the so called "command line", i.e. a terminal where commands can be entered in.

In this computer course, we will first restrict to the visual interface that is installed on your computers, which is the Gnome desktop.

- Read additional infos PDF!
- Power on your lab computer, switch to Linux, use Gnome, navigate, create folders etc.

## 2 Revision: Model of crystal structures

In solid state physics, probably the most essential concept is the one of crystalline systems. The main property of a crystal is its symmetry. Virtually all other physical properties can be deduced from it. From a mathematical point of view, crystallography is basically nothing but applied group theory.

In this course, we want to have a look at some specific types of crystals which are highly symmetric and thus easy and quick to compute. But first some recap of what you should already know. Think about the Diamond structure:

1. What basic crystal lattice is behind this structure? What else can you tell about that crystal?
2. What other compounds that crystallize in this system do you know?
3. Are there any other important basic structures that you know of?
4. How many atoms does the fcc, bcc and diamond unit cell contain? Draw them (without basis)!
5. What is the difference between a conventional and a primitive cell? How can the primitive fcc cell be built in terms of the crystal axes of the conventional fcc cell? What changes for bcc?
6. What can you tell about the edge length and the volume of the primitive cell in relation to the lattice constant, which is defined as the edge length of the conventional cell?

## 3 Crystals and their visualization

Compared to purely (group) theoretical approaches, in computational physics it is often necessary to first study new systems visually. We usually use one of these tools for that purpose:

- VESTA, XCrysDen, ASE-gui, jMol, ovito (and others)

Before we can look at a crystal structure, we first have to find a description of the crystal setup. A standardized format for that kind of information is given with CIF - the Crystallographic Information File format. The details of this format are not so important, but we will have a short look at the content of such a file nevertheless.

**Choose a material:**

| Diamond | Zincblende | Rocksalt |
|---|---|---|
| C, Si, Ge | ZnS, GaAs, AlP, SiC | NaCl, LiF |

**Tasks:**

1. Download a Crystallographic Information File (CIF) for your system:
   - Inorganic Crystal Structure Database: `https://icsd.fiz-karlsruhe.de` (only accessible from within university network or via demo account)
   - Crystallography Open Database: `http://www.crystallography.net`
2. Open the file in VESTA (pre-installed on pool computers) and have a look at the 3D model.
3. Identify atom positions and species.
4. Find lattice constants and space group.
5. Extend the view to a 4x4x4 grid of unit cells. Look at the crystal from different perspectives, try to detect familiar symmetries, then undo the changes.
6. Identify symmetry equivalent atoms using Wyckoff positions and compare with Bilbao Server results for your space group:

   Bilbao Server | Bilbao Server - Wyckoff Positions | Bilbao Server - SG 227 with Cell Choice 1
7. Try different options under `Edit` → `Bonds...` (Ctrl+B), in particular the "Do not search atoms beyond the boundary" setting.
8. Reduce Boundaries to 0.09 (Ctrl+Shift+B).
9. Convert conventional into primitive cell and verify it has the correct volume.
   `Edit` → `Edit Data` → `Unit Cell` → `Transform…` → `Rotation Matrix P`
10. Reproduce the original conventional cell
11. Run the spglib_wyckoff.py script. Compare its output with the cell parameters, atom positions and Wyckoff positions with data from VESTA and Bilbao Server. What is the purpose of the ICT standardized cell?