student summaries and exam question suggestions
Crystallography

These pages contain student summaries for the module **Crystallography**, *as well as student suggestions for exam questions on this module. You can use these pages as a study help for this module. The summaries can help you to see the highlights of this module from different points of view. The questions can challenge you to think about the content. If you take the exam, then some of the questions suggested this year will be included in the exam. The contributions suggested this year are* are printed in color. *The ones in black were contributed in previous years.*

1. student summaries

- How to understand, make and edit CIF files
- Crystal Structures
- There are many terms in crystallography with different definitions that are all important to distinguish and know.
- This was a very practical chapter in which we spoke about where to find CIF files and how to pick the correct one out of the options provided for a certain molecule. We then looked at what's inside these files and how to read the information contained inside. We defined concepts as space group and Wyckoff positions and the influence these have on the crystal. Finally we learned how to construct CIF files ourselves for simple crystals and discussed some online tools that can help in the construction and visualiation of these files.
- How to read a cif file. How to find cif files. How to utilize tools to measure and view the crystal desribed by a cif file.
- Crystal structure are codified with their space group, cell unit and Wyckoff positons. CIF files allow us to easily carry the information about these structures into visualization and computational tools.
- - CIF repositories - Converting CIF to input file
- The symmetry handling of crystal structure, that is, the definition of a space group, Wyckoff positions, and their relation to a unit cell's appearance, should be taken home.
- How to read and convert CIF files
- How to convert cif files.
- 1. In which way the data of a crystal is stored on web, and how do we read it. (That is, by a .cif file or any other format)

  2. How much information that file contains and how to manually work with some of it (pen and paper calculation).

  3. How to convert some of these file extensions to the other forms and what are the programs they are compatible with.

  4. Creating a .cif file from scratch.
- What a cif file is and what the minimum amount of information is that it has to contain. Know what Wyckoff positions are and their use in cif files. How symmetry is used to minimize the amount of atomic coordinates needed in a cif file.
- CIF files are standard files to write down properties of crystals. You can convert these to input files of your DFT code. Calculations are simpler when you know the space group of the crystal. The nuclei are located at certain Wyckoff positions of this spacegroup.
- A cif file is a convenient almost universal tool to convey crystallographic information.
- A CIF file is a universal file that is used to specify a particular crystal. To specify the crystal you must give the space group, Wyckoff positions, lattice parameters and values of free coordinates. You can find this required information about a particular crystal using the Open access crystallography data base and the Bilboa crystallographic server.

- cif format is a global format for multiple dft programs
- Cif files - how to read them (cell parameters, coordinates, wyckoff positions of atoms), how to create cif files with symmetry information "from scratch"
- We learned to search for and view the Crystal structure via cif files. We have created a cif file and converted it into QE input
- characteristics of crystal in order to obatin information about it and how to search and introduce those characteristics into QE

2. exam question suggestions

- Explain the concept of Wyckoff positions and their link with symmetry
- What is cif files and how we use it
- Give the types of crystal systems (eg. FCC, face cubic centered)
- Provided an image of a CIF file containing the necessary information: How many geometrical degrees of freedom does this crystal have?
- (Provide a cif file with some basic information in it) Try to derive as much as possible from this cif file, try to draw the crystal (provided it isnt incredible complex).
- Which information does a CIF file contain?
- What do you understand by a space group of a crystal? What other information may you need to draw a unit cell of a given crystal structure?
- Given a cif cile, how many degrees of freedom does this crystal have?
- Give a way to add symmetry to the cif files.
- Working with the Wyckoff positions, figure out all other atom coordinates when only one coordinate is given.
- What is the relation between space group, unit cell and Wyckoff positions. Can you fully define a crystal with only two of those? Explain why or why not.
- What are Wyckoff positions?
- Explain briefly what a cif file is and why it is said to be 'human-readable'
- What is contained in a CIF file?
- using the cell parameters of a hexagonal lattice, identify lattice constant c, provided a value of lattice parameter a
- How does the symmetry group influence the structure of the cif file?
- Name the most important features of a cif file
- How would the asymmetric unit affect the calculation efficiency? Is that considered by the code to construct the full unit cell
- Which parameters define the structure of a crystal?