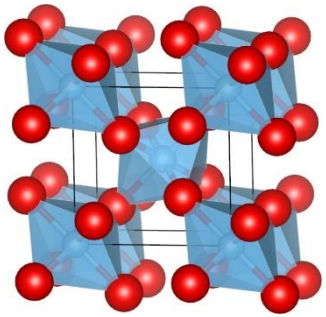
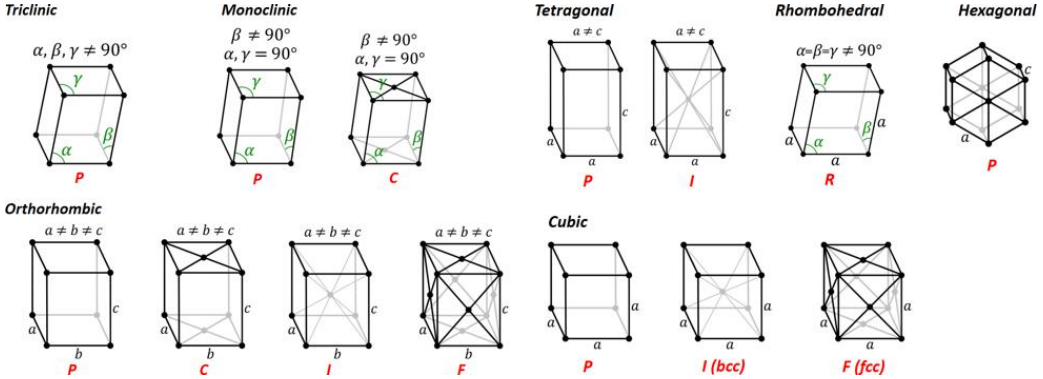
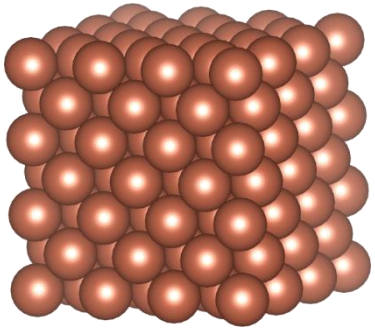
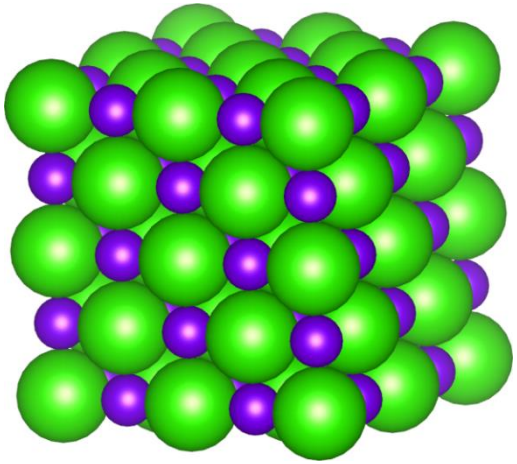
Solid State Chemistry: Summary



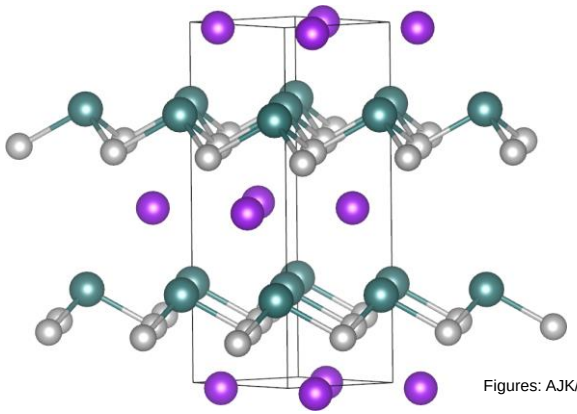






FIZ Karlsruhe ICSD

COD



Figures: AJK/Wikipedia/FIZ/COD

There is no new content here, just reflections on the course topics

Review of learning outcomes

After the course the student will be able to

1. Apply the basic concepts of structural chemistry, such as unit cell, lattice parameters, crystal system, and space group.
2. Search crystal structures of inorganic solid-state compounds from databases, analyze and visualize the crystal structures.
3. Analyze bonding in solid state chemistry: Electronegativity, radii and packing of atoms, ligand field theory, band theory.
4. Describe synthesis methods used in solid state chemistry and read the information given in various phase diagrams.
5. Analyze information from various structure characterization methods and utilize powder X-ray diffraction data for phase identification.
6. Explain basic structure-property correlations of various inorganic materials.

Let's review the course contents briefly

Learning outcomes review (1)

- Apply the basic concepts of structural chemistry, such as unit cell, lattice parameters, crystal system, and space group.
  - It really isn't possible to pass the course without understanding these!
  - Large number of practical exercises throughout the course

- Search crystal structures of inorganic solid-state compounds from databases, analyze and visualize the crystal structures.
  - Key practical skills from the exercises:
    1. Finding a correct structure from a database like ICSD or COD
    2. Being able to visualize that structure with VESTA or Jmol
    3. Being able to describe the structure based on the visualization (coordination polyhedra etc.)

Learning outcomes review (2)

- Analyze bonding in solid state chemistry: Electronegativity, radii and packing of atoms, ligand field theory, band theory.
  - Electronegativity was used as a convenient descriptor throughout the course.
  - The various atomic and ionic radii were discussed and their usage in understanding some structural aspects was highlighted. Still, the radii should be considered only as a helpful tool, but not a real physical fact.
  - Close packing was discussed in detail and in relation to many structures (close-packing of metals, close-packing of anions)
  - Crystal and ligand field theory were discussed in detail, including Jahn-Teller effect. Several exercises within this theme and this was also our introduction to magnetism
  - Band theory of solids was discussed in a qualitative way and we practiced the qualitative interpretation of band structure diagrams. More details in the computational chemistry courses.
    - Or maybe carry out a research project in computational solid state chemistry? Contact Antti if you are interested.

Learning outcomes review (3)

- Describe synthesis methods used in solid state chemistry and read the information given in various phase diagrams.
  - A number of synthesis methods was discussed in the lecture slides, but instead of learning them by heart, the main goal was to have an overall idea of the wide variety of synthesis methods available.
  - Phase diagrams were introduced from a practical point of view, we did not put so much emphasis on the theoretical aspects.
- Analyze information from various structure characterization methods and utilize powder X-ray diffraction data for phase identification.
  - A number of structure characterization methods were discussed, but instead of learning them by heart, the main goal was to have an overall idea of the wide variety of characterization methods available.
  - Interpretation of vibrational spectra based on quantum chemical calculations. This option may be good to keep in mind if you have spectra to interpret
  - Phase identification was a key concept and was practiced in a number of exercises. We did not use the big commercial databases for phase identification, but had some practice with the open access Powder COD –tool.

Learning outcomes review (4)

- Explain basic structure-property correlations of various inorganic materials
  - The course included an overview of the most common structure types, and many individual materials were discussed
  - Basic electronic properties (insulator/semiconductor/metal) have been discussed.
  - Effects of defects and doping on the properties were discussed during the last week of the course.
  - Correlation of bonding and hardness was highlighted for a series of minerals.
  - Properties and applications of solid-state materials are discussed in detail on the course CHEM-E4215 Functional Inorganic Materials (Fall term, period I)

Summary

- If I would need to pick one word that summarizes this course, it would be **structure**
- I also hope that the rather large number of different compounds discussed on the course gave you an overview on the versatility of solid state chemistry
- I thank you for your active participation so far and the course still continues with the Wiki project!