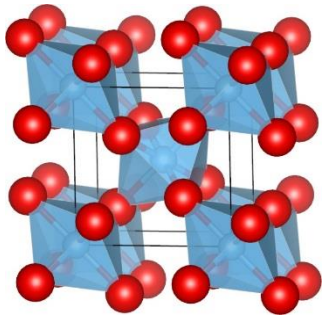
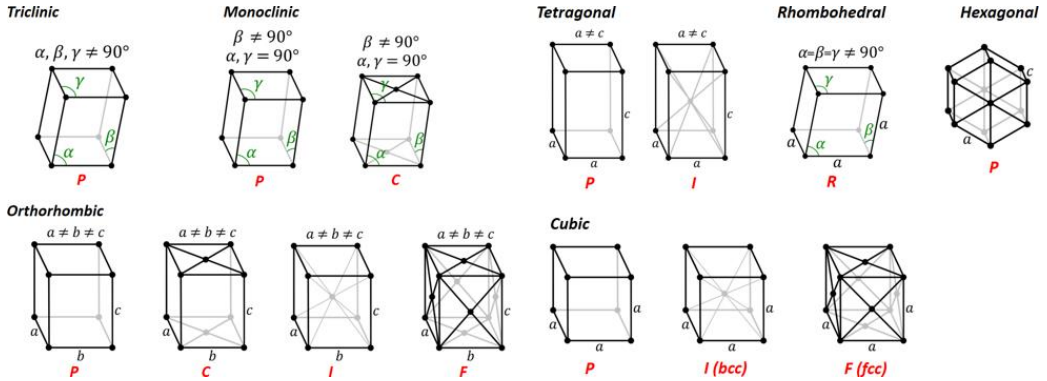
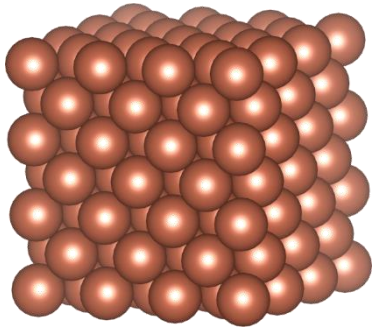
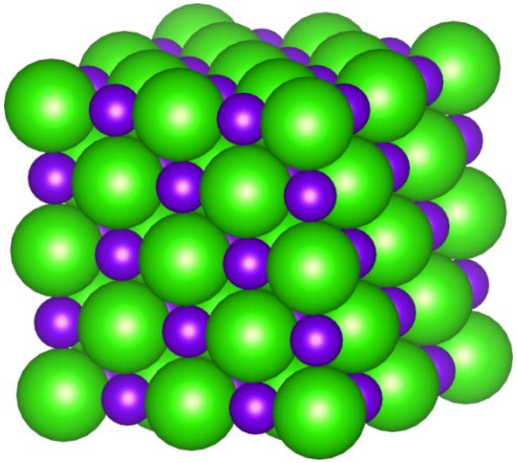
Lecture 16: Summary



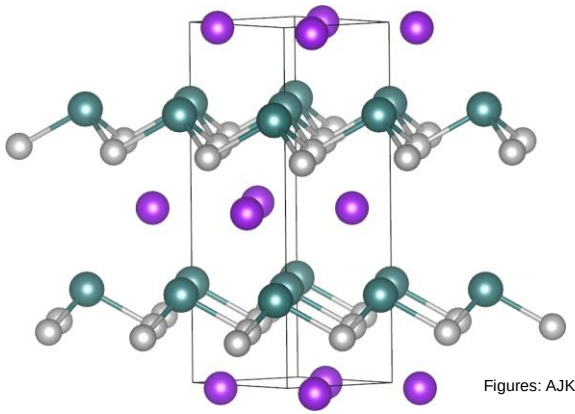






FIZ Karlsruhe ICSD

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. Describe the roles of crystal defects, doping, and non-stoichiometry
7. 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!
  - We had several practical exercises about point groups
  - Recognizing the crystal system from the lattice parameters and the symmetry elements is a useful skill
  - Space groups were introduced, but these are not as easy to deduce from the structure as molecular point groups.
- 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.)
  - Based on your work in the exercises and the Wiki project, I can say with confidence that this learning outcome has been fulfilled

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.
  - Effective nuclear charge was discussed as one concept behind the electronegativity (but it was not enough to explain EN completely)
  - 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
  - The band theory was discussed in a qualitative way and we practiced the qualitative interpretation of band structure diagrams. More details in the computational chemistry courses (or in 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 and this was also one focus of the Wiki projects.
  - 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 and these were also a focus of the Wiki projects
  - 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)

- Describe the roles of crystal defects, doping, and non-stoichiometry
  - Defects and doping (of semiconductors) were discussed on two lectures. The thermodynamics of defect formation was one of the key concepts
  - Non-stoichiometry (of oxide materials) was only discussed briefly
- 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 a lot. Electrical conductivity was also discussed a bit in the case of semiconductors.
  - Correlation of bonding and hardness was highlighted for a series of minerals
  - There was not much emphasis on properties, but structure-property aspects such as layered Li ion battery materials or functional perovskite materials were discussed.
  - For more emphasis on the material properties and their applications: CHEM-E4215 Functional Inorganic Materials (Fall term, period II)

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!

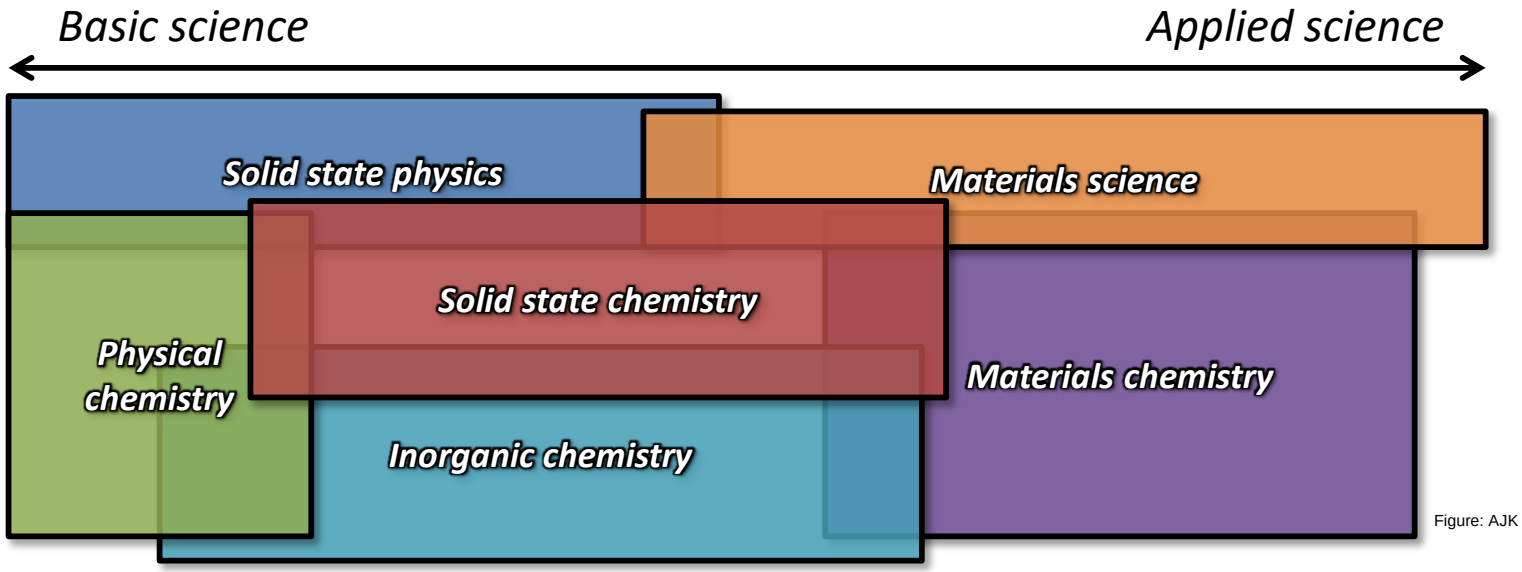


Figure: AJK