

Crystal Chemistry

The course discusses the study of inorganic crystalline solids. The crystal structures of the elements, binary, ternary and modular compounds is presented. Correlation between electronic structure and crystal structure using the LCAO approach. Defects in crystals and how those affect the physical properties of the solids (semiconductors, scintillators, transparent conducting oxides, etc.). Methods of crystal growth and structural characterization with X-ray diffraction. Modern technological applications of inorganic materials. The main educational goals that the students will achieve upon completion of the course include:

1. **The structure of solids:** Description and classifications of crystals through polyhedral representations of inorganic crystal structures.
2. **Band structure:** Electronic structure derived from crystal structure. Structure-property relations.
3. **Non-stoichiometry and defects in crystals:** Manipulation and control of the physical properties of solids.
4. **Synthetic methods and characterization in inorganic solids:** Crystal Growth of single-crystals, polycrystalline and amorphous solids
5. **Application of Inorganic compounds in technology**

Syllabus:

1. Structure types of Solids

- α) Metals and Nonmetals
- β) Binary compounds: AB , AB_2 , AB_3 , A_2B_3 , A_xB_y
- γ) Ternary compounds: ABX_2 , ABX_3 , AB_3 , AB_2X_4 , A_2BX_4 , AB_2X_2
- δ) Intermetallics and Zintl Phases
- ε) Modular compounds: Polytypes, Homologous series and misfit layered compounds

2. Band structure (based on R. Hoffmann review).

- α) Constructing “Spaghetti” diagrams starting from molecular orbitals.
- β) Electronic instability (Peierls distortion, Jahn-Teller effect)
- γ) Density of states, band folding, direct and indirect bandgap
- δ) Quantum confinement: Low-dimensional materials, Quantum wells, Quantum wires, Quantum dots

3. Non-Stoichiometry and Defects in Crystals

- α) Nonstoichiometry and diffusion. Thermal quenching, sintering, and annealing.
- β) Phase diagrams, eutectics, spinodal decomposition and solid solutions.
- γ) Phase transitions. Phase transitions in inorganic solids, crystals and amorphous solids.

4. Synthesis methods

- α) Solid-state synthesis, wet synthesis, solvothermal synthesis
- β) Crystal Growth
Growth from melts, solutions and vapor transport.

γ) Structural characterization

Structure determination from single-crystals and crystalline powders. Characterization of amorphous solids (Pair Distribution Functions (PDF))

5.Applications of Inorganic Compounds in Modern Era Technology

- *Inorganic Semiconductors in Optoelectronics*

Photodiodes in Photovoltaics, Detectors and LED's

- *Porous Materials*

Gas Separation and Catalysis

- *Hydrogen Technology*

Production, Storage and Reactivity

- *Energy Storage*

Solid State Batteries

Evaluation: Successful completion of the course involves the writing of a scientific manuscript in English (40%) (JACS Communication format) on a topic related with the technological application of inorganic materials, and its oral presentation in the class (40%). The remaining (20%) is evaluated based on the class participation and understanding throughout the course. The topic will be chosen by the student after consultation with the instructor.

Bibliography:

- *Suggested bibliography:*

- 1) [Ulrich Müller, «Inorganic Structural Chemistry», 2nd Edition, Wiley 2006.](#)
- 2) Alexander F. Wells, «*Structural Inorganic Chemistry*», 5th Edition, Oxford University Press 1984.
- 3) Roald Hoffmann, «*How Chemistry and Physics Meet in the Solid State*», *Angew. Chem. Int. Ed. Engl.* (1987) 846-878
- 4) Anthony R. West. «*Solid State Chemistry and Its Applications*», 2nd Edition, Wiley 2014.
- 5) Richard J. D. Tiley, «*Defects in Solids*», Wiley 2008
- 6) Giovanni Ferraris, Emil Mackovicky, Stefano, Merlino, «*Crystallography of Modular Materials*», IUCr 2004.
- 7) Erwin Parthé «*Crystal Chemistry of Tetrahedral Structures*» CRC Press 1964

- *Related Scientific Journals:*

[Chemistry of Materials](#)

[Materials Horizons](#)

[Nature Materials](#)

[Advanced Materials](#)

[Journal of Solid State Chemistry](#)