CHEM-E4205: Crystallography Basics & Structural Characterization (5 cr)

The course deals with **crystal chemistry** concepts and structural **characterization** techniques of **inorganic materials** and covers also the basics of **crystallography**. The emphases are on the various diffraction and spectroscopic methods used for phase identification, **crystal structure** determination and studies of **chemical environment**.

Time Slots	**Tuesday 12–14, Friday 10-12 & Friday 14–16**
Lectures	Lectures in Zoom; lecture slides and additional reference material (if needed) provided in MyCourses before the start of each lecture.
Exercises	Last part of Friday hours (Zoom or Classroom D422): to explain the assignments & give some guiding. Exercise answers returned by next Monday 6 pm.
Seminars	Given individually on an assigned topic
Teachers:	Maarit Karppinen Eeva Rautama (Rietveld) Sami Vasala (Synchrotron & XAS & RIXS) Ramin Ghiyasi (XRR)

SCHEDULE

		Date	Topic
1.	Tue	14.09.	Lec-1: Introduction
2.	Fri	17.09.	Lec-2: Crystal Chemistry & Tolerance parameter
3.	Fri	17.09.	EXERCISE 1
4.	Tue	21.09.	Lec-3: Crystal Chemistry & BVS
5.	Fri	24.09.	Lec-4: Symmetry & Point Groups
6.	Fri	24.09.	EXERCISE 2
7.	Tue	28.10.	Lec-5: Crystallography & Space Groups
8.	Fri	01.10.	Lec-6: XRD & Reciprocal lattice
9.	Fri	01.10.	EXERCISE 3
10.	Tue	05.10.	Lec-7: ND & GI-XRD
11.	Fri	08.10.	Lec-8: Rietveld
12.	Fri	08.10	EXERCISE 4: Rietveld
13.	Tue	12.10.	Lec-9: Synchrotron radiation & XAS & RIXS
14.	Fri	15.10.	Lec-10: EXAFS & Mössbauer
15.	Fri	15.10.	EXERCISE 5
16.	Tue	19.10.	Seminars: XPS, FTIR, Raman, ED, HRTEM, SEM, AFM
17.	Fri	19.10.	Lec-11: XRR
18.	Fri	22.10.	EXERCISE 6: XRR

COURSE START:
Tue 14.09. at 12.15
in Zoom

EXAM:
Fri Oct. 29, 2021

GRADING (max 100 points)

- Exam: 0 – 44 points
- Exercises: = 0 – 36 (= 6 x 6) points
- Seminar (mandatory): 10 – 20 points

INSTRUCTIONS for SEMINAR PRESENTATION/REPORT

- Topics: **IR, Raman, XPS, SEM, AFM, HRTEM, ED, EELS**
- Seminar presentation is mandatory
- Given individually
- Evaluated in the scale: 10 ~ 20 points
- Presentation is given in English, and the slides will be put up in MyCourses afterwards
- Presentation: 25+5 minutes
- Rough content of the presentation/report:
  - principle of the technique
  - type of information gained
  - interpretation of the measured data
  - pros & cons
  - two to three research examples
    (you will be given some relevant research papers for an example)

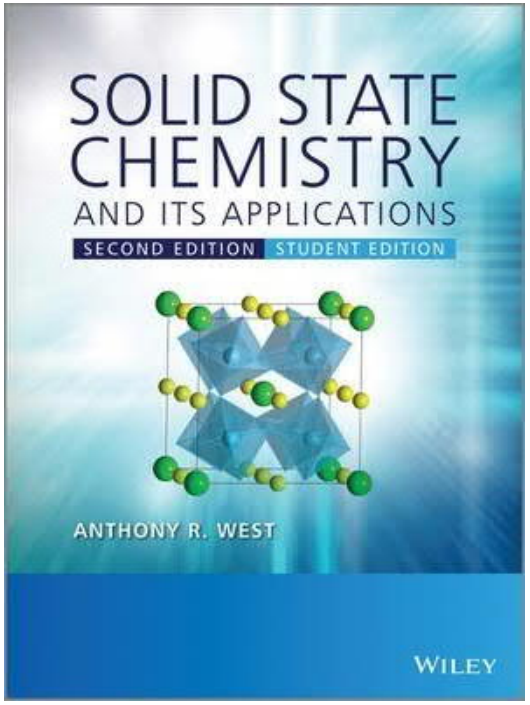
TEXT BOOKs & Background Knowledge

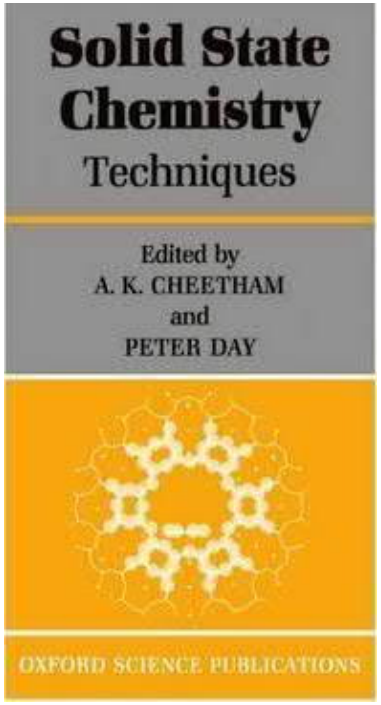
This course does not follow any specific text book; no text book fully covers the topics included; below are examples of text books which could be useful reference/background books for many of the course topics.

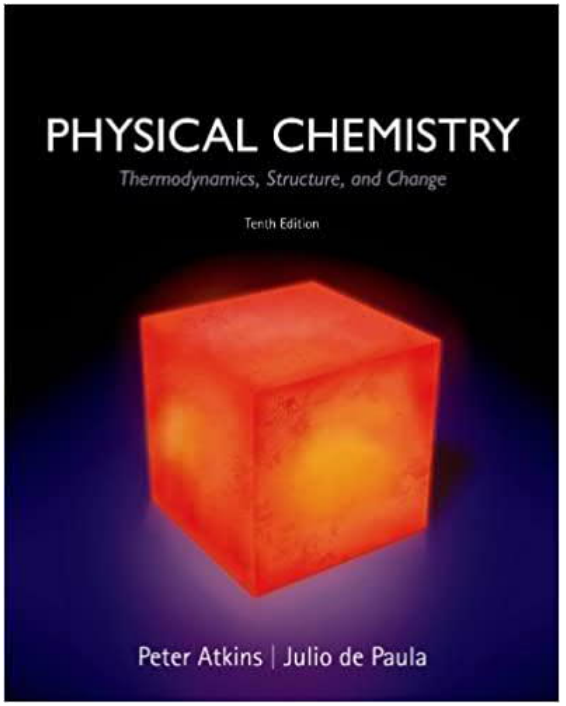
Although the following two courses are not mandatory prerequisites, it maybe difficult to follow this course without a similar basic background knowledge on inorganic (materials) chemistry and solid state chemistry:

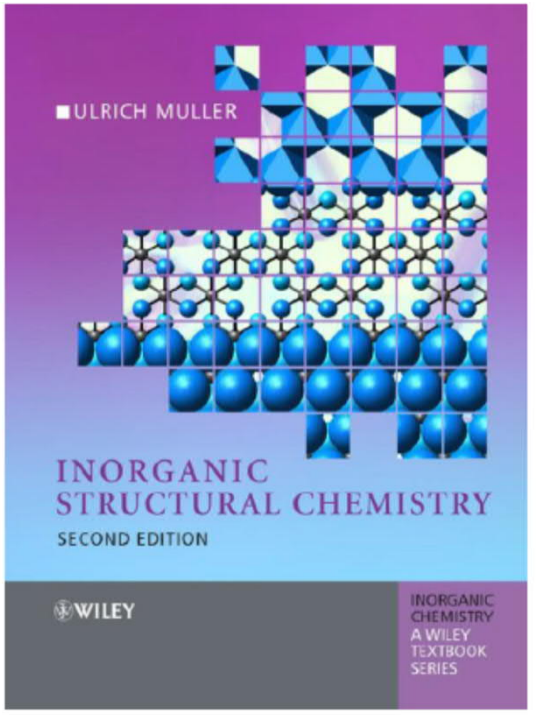
CHEM-E4130: Chemistry of Elements (Maarit Karppinen)

CHEM-E4155: Solid State Chemistry (Antti Karttunen)









LEARNING OUTCOMES

After the course the student will be able to

1. use symmetry elements for the description of the symmetries of molecules and crystals
2. determine the point group for a molecule
3. read the space group symbols so as to understand the information provided by the symbol
4. draw unit cells once the space group, lattice parameters, and atomic coordinates are known
5. explain the diffraction phenomenon
6. explain the steps in crystal structure determination and the principles of Rietveld refinement; evaluate the feasibility of a crystal structure model based on a bond valence sum (BVS) calculation
7. understand the interplay with structural features/chemical state
8. explain the principles of the most important structural characterization techniques and understand and critically evaluate the information revealed by the techniques for inorganic materials
9. select the most suitable technique(s) for each specific structure-related research problem

The course deals with structural characterization techniques of **inorganic materials** and covers also the basics of crystallography. The emphases are on the various diffraction and spectroscopic methods used for phase identification, **crystal structure** determination and studies of **chemical environment**.