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

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**.

"Lectures"	Friday 10.15 – 12.00 & Friday 14.15 – 16.00 "Lectures" are mostly studied **indipendently** by reading the lecture slides and (if needed) additional reference material (given or found).
Exercises	Assignment given on each Friday, answer returned by next Friday.
"**Tutorials"**	Preferably on Tuesdays between 10–17 (other days can be agreed too); Students have a possibility to reserve (individually or in small groups) a time slot (30 min) for a weekly tutorial to clarify questions which remained nonunderstood from the written lecture slides/reference literature; Tutorials are not mandatory; Tutorials are held in Maarit's office or in **Teams**.
"Seminars"	**Seminar** given individually or in small groups (1-3) on an assigned topic. Alternatively, a short **written report** on the same topic.
Teachers:	Maarit Karppinen Eeva Rautama (Rietveld) Ramin Ghiyasi (XRR)

SCHEDULE

	Date		Topic
1.	Fri	11.09.	Course Introduction
2.	Fri	11.09.	Crystal Chemistry & BVS
			EXERCISE 1
	Tue	15.09.	TUTORIAL
3.	Fri	18.09.	Symmetry & Point Groups
4.	Fri	18.09.	Crystallography & Space Groups
			EXERCISE 2
	Tue	22.09.	TUTORIAL
5.	Fri	25.09.	XRD
6.	Fri	25.09.	ND
			EXERCISE 3
	Tue	29.09.	TUTORIAL
7.	Fri	02.10.	Rietveld
			EXERCISE 4: Rietveld
8.	Fri	09.10.	EXAFS & XANES
9.	Fri	09.10.	Mössbauer
			EXERCISE 5
	Tue	13.10.	TUTORIAL
10.	Fri	16.10.	GI-XRD & XRR (thin film techniques)
			EXERCISE 6: XRR
	Tue	20.10.	Seminars: XPS, FTIR, Raman,ED, HRTEM, SEM, AFM

COURSE START:
Fri 11.09. at 10.15
in Zoom

EXAM:
Thu Oct. 22, 9:00-13:00

GRADING (max 100 points)

- Exam: 44 points
- Exercises: 6 x 6 = 36 points
- Seminar or written report: 20 points

INSTRUCTIONS for SEMINAR PRESENTATION/REPORT

- Topics: **IR, Raman, XPS, SEM, AFM, HRTEM, ED, EELS**
- Presentation is given individually or preferably in a group of two or three persons; in case it is a group effort, it is recommendable to cover two related techniques, e.g. IR + Raman
- Alternatively, it is also possible to write a report on the topic
- Seminar/report will be evaluated in the scale: $0 \sim {}_{20}$ points
- The presentation is given (report written) in English, and the slides will be put up in MyCourses afterwards
- Presentation: 25+5 minutes; Report: 5-7 pages
- 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)

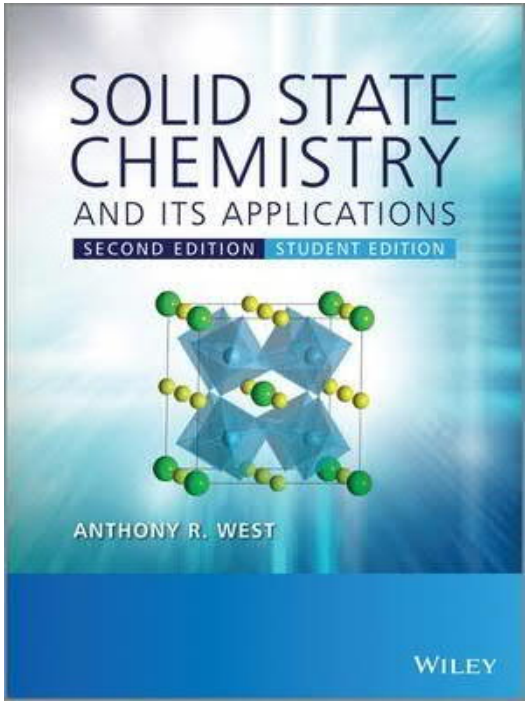
TEXT BOOKs & Background Knowledge

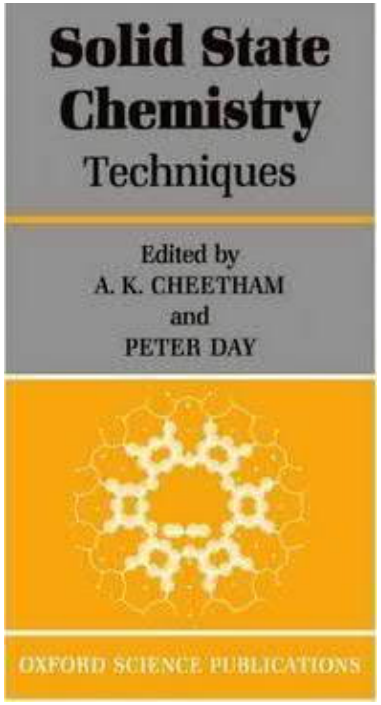
This course does not follow any specific text book; no text book fully covers the topics included; below are examples of text books which could be useful reference/background books for many of the course topics.

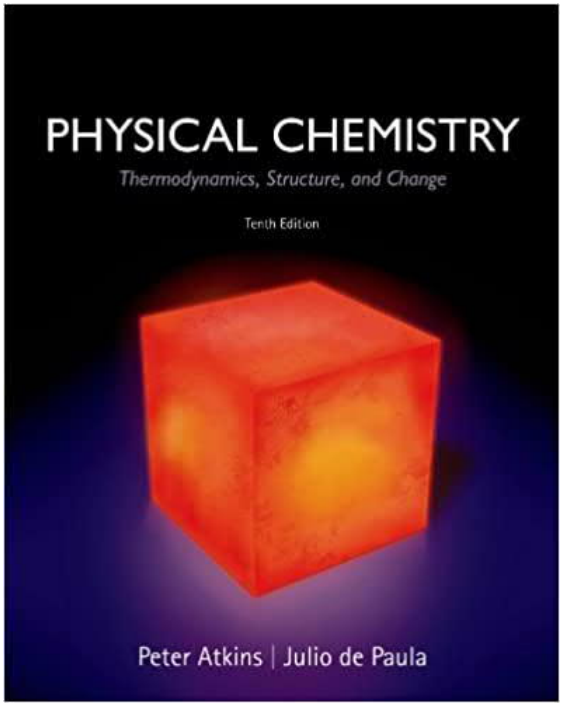
Although the following two courses are not mandatory prerequisites, it maybe difficult to follow this course without a similar basic background knowledge on inorganic (materials) chemistry and solid state chemistry:

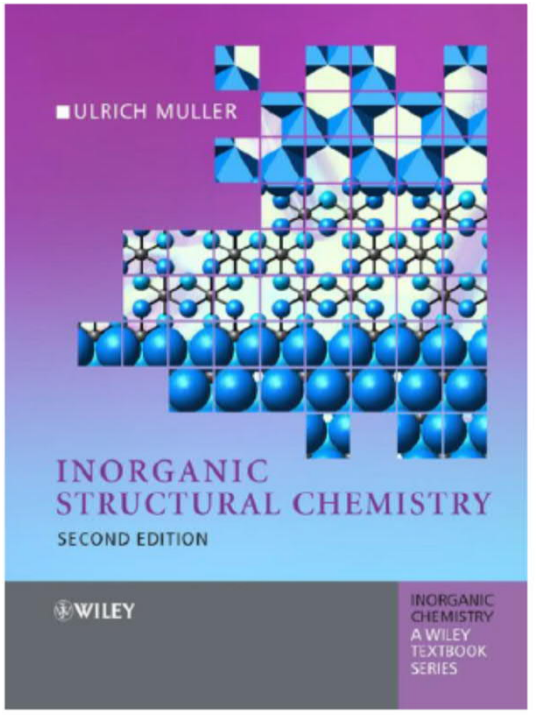
CHEM-E4130: Chemistry of Elements (Maarit Karppinen)

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. explain the principles of the most important structural characterization techniques and understand and critically evaluate the information revealed by the techniques for inorganic materials
8. select the most suitable technique(s) for each specific structure-related research problem

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