Modulbezeichnung:	**Modern X-ray Structure Determination (MXD)** (Modern X-ray Structure Determination)	**5 ECTS**
Modulverantwortliche/r:	Frank Wilhelm Heinemann	
Lehrende:	Frank Wilhelm Heinemann	

Startsemester: WS 2021/2022	Dauer: 1 Semester	Turnus: halbjährlich (WS+SS)
Präsenzzeit: 45 Std.	Eigenstudium: 105 Std.	Sprache: Englisch

Lehrveranstaltungen:

Modern X-ray structure determination of single crystals (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Frank Wilhelm Heinemann)

Inhalt:

- Fundamentals of crystallization and polymorphism
- Structural description of single crystals, crystal systems, unit cell, symmetry and symmetry elements, space groups
- Diffraction power of crystals, diffraction conditions, structure factor
- Generation of X-rays, single crystal diffractometers, detection techniques
- Structure solution techniques and refinement procedures, software, problems and pitfalls, interpretation of results
- Anomalous dispersion and absolute structure
- Graphical representations, use of data bases

Lernziele und Kompetenzen:

Students ...

- get insight into thermodynamics of crystallization and crystallization techniques
- get fundamentals of the theory behind crystal structure determination
- get practice in crystal selection, mounting and measurement set-up
- get hands-on training in structure solution and refinement using up-to-date software
- are enabled to interpret and compare results of a single crystal structure determination

Literatur:

- Werner Massa: Kristallstrukturbestimmung. Teubner Studienbücher Chemie, Vieweg und Teubner, 6. Auflage, 2009, ISBN: 3834806498
- William Clegg: Crystal Structure Determination. Oxford Chemistry Primers. Oxford University Press, 1998, ISBN: 0198559011
- Further literature will be recommended in the course

Studien-/Prüfungsleistungen:

Modern X-ray Structure Determination (Prüfungsnummer: 65581)
Prüfungsleistung, Übungsleistung
Anteil an der Berechnung der Modulnote: 100%
weitere Erläuterungen:
Lab report in manuscript style (max. 2000 words plus raw data); module is ungraded, but has to be passed!
Prüfungssprache: Englisch

Erstablegung: WS 2021/2022, 1. Wdh.: keine Angabe
1. Prüfer: Frank Wilhelm Heinemann

Organisatorisches:

- Module can be taken in winter or in summer term
- Students have to register for the module examination (check registration periods)
- Information/registration available on studon

Bemerkungen:

Module campatibility:

- as Elective Module in M.Sc. Chemistry or M. Sc. Molecular Science (5 ECTS, not graded)