

Modulbezeichnung: Symmetry and Group Theory (SGT) **5 ECTS**
(Symmetry and Group Theory)

Modulverantwortliche/r: Jörg Libuda

Lehrende: Jörg Libuda, u. Mitarbeiter

Startsemester: WS 2021/2022

Dauer: 1 Semester

Turnus: jährlich (WS)

Präsenzzeit: 45 Std.

Eigenstudium: 105 Std.

Sprache: Englisch

Lehrveranstaltungen:

Seminar Symmetry and Group Theory - Applications in Chemistry, Physics and Material Sciences (WS 2021/2022, Seminar, 1 SWS, Jörg Libuda et al.)

Symmetry and Group Theory - Applications in Chemistry, Physics and Material Sciences (WS 2021/2022, Vorlesung mit Übung, 3 SWS, Jörg Libuda)

Inhalt:

- Symmetry of Molecules (symmetry elements, operations, point groups, notations)
- Symmetry of Crystals, Surfaces and Interfaces (symmetry in 1, 2 and 3 dimensional periodic structures, lattices, crystal classes, space groups)
- Compact Course Group Theory (elements group theory, definitions, reducible and irreducible representations, orthogonality theorem, character tables)
- Group Theory and Quantum Mechanics (representations, operators and symmetry, matrix elements, direct product functions, projection operators)
- Symmetry of Organic Molecules: From Electronic Structure to Reactivity (symmetry adaption, cyclic groups, many electron systems, electronic transitions, configuration interaction, symmetry controlled reactions)
- Symmetry in Anorganic Chemistry: From Atoms to Complexes (MO models, transition metal complexes, direct product groups, rotation inversion group, angular momentum coupling, crystal field splitting, vibronically allowed transitions)
- Symmetry and Spectroscopy: Vibrational Spectroscopies (analysis of vibrational modes, normal coordinate analysis, symmetry of vibrational wave functions, vibrational spectroscopy, selection rules)
- Symmetry in Crystal Physics: Tensor Description of Physical Properties (tensors, axial, polar, representations, transformation properties, intrinsic symmetry, Neumann's principle, Curie's principle)
- Symmetry and Electronic Structure of Solids: Band Structures (translation group and irreps, reciprocal lattice, k-space, Bloch functions, Brillouin zones, symmetry of bands)

Lernziele und Kompetenzen:

Students

- acquire detailed understanding how to use symmetry properties and the mathematical tools of group theory in a broad range of application fields in chemistry, physics and materials science.

Verwendbarkeit des Moduls / Einpassung in den Musterstudienplan:

Das Modul ist im Kontext der folgenden Studienfächer/Vertiefungsrichtungen verwendbar:

[1] **Chemistry (Master of Science): ab 1. Semester**

(Po-Vers. 2020w | NatFak | Chemistry (Master of Science) | Wahlmodule | Symmetry and Group Theory)

Dieses Modul ist daneben auch in den Studienfächern "Molecular Science (Master of Science)" verwendbar.

Studien-/Prüfungsleistungen:

Symmetry and Group Theory (Prüfungsnummer: 65461)

Prüfungsleistung, mündliche Prüfung, Dauer (in Minuten): 20

Anteil an der Berechnung der Modulnote: 100%

weitere Erläuterungen:

O20(PL): Oral Examination (20 minutes) or alternativ examination according to FAU Corona Statutes, Date by agreement

Prüfungssprache: Englisch

Erstablingung: WS 2021/2022, 1. Wdh.: WS 2021/2022

1. Prüfer: Jörg Libuda

Organisatorisches:

- lecture module will be taught **online** (synchronous)
- lecture module will be offered only in winter term
- Students have to register for the module (check registration periods)
- Registration/further information via **StudOn**

Bemerkungen:

Module compability:

- lecture module can be taken as part of the Elective module (5 ECTS, not graded)