The Hebrew University of Jerusalem

Syllabus

MATHEMATICS METHODS IN CHEMISTRY (5) - 69834

Last update 24-01-2024

HU Credits: 3

Degree/Cycle: 2nd degree (Master)

Responsible Department: Chemistry

Academic year: 0

Semester: 1st Semester

Teaching Languages: English

Campus: E. Safra

Course/Module Coordinator: Prof. Hardy Gross

Coordinator Email: hardy@mpi-halle.mpg.de

Coordinator Office Hours: By appointment

Teaching Staff:

Prof. Eberhard (Hardy) Gross

Course/Module description:

Introduction to the theory of complex functions and to the basics of functional analysis

Course/Module aims:

To give the students insight in the properties of holomorphic functions, to familiarize them with the different types of singularities and their significance in spectroscopy, and to teach the basic concepts of functional analysis and variational calculus

Learning outcomes - On successful completion of this module, students should be able to:

Students should be able to perform complex contour integrals, and to apply Kramers-Kronig relations in spectroscopy. They should be able to evaluate the functional derivative of any functional.

Attendance requirements(%):

Attendance is not compulsory, but is expected and recommended

Teaching arrangement and method of instruction: Frontal lecture, via zoom.

Course/Module Content:

- *Complex numbers*
- *Holomorphic functions*
- *Cauchy's theorem*
- *Cauchy's integral formulae*
- *Residue theorem*
- *Multi-valuedness, the Riemann surface, and its relation to the molecular wave function*
- *Taylor series*
- *Laurent series*
- *Classification of singularities*
- *Optical spectra as poles of the response function*
- *Causality and Kramers-Kronig relations*
- *Functionals*
- *The functional derivative*
- *variational principles*

Required Reading:
None

Additional Reading Material:
George B. Arfken, Hans J. Weber and Frank E. Harris: Mathematical Methods for Physicists: A Comprehensive Guide (Academic Press, 2012)

Grading Scheme:
Essay / Project / Final Assignment / Home Exam / Referat 100 %

Additional information: