

CHEM 505. COMPUTER MODELING OF MOLECULES AND MATERIALS.

Credits: 3

Offered by: Chemistry (Faculty of Science)

Terms offered: Winter 2026

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Description

A comprehensive introduction to computational methods and software for graduate students and advanced undergraduates. The main focus of the course is on important practical aspects of chemistry-related computer modeling: how to perform simulations reliably and efficiently, and how to interpret simulation results. Two main classes of computer simulations--electronic structure methods and statistical mechanics methods--will be discussed in detail together with a wide range of chemical examples.

- Prerequisite(s): CHEM 345 or equivalent and CHEM 365 or PHYS 329 or equivalent, and COMP 202 or COMP 208 or equivalent.

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