

COURSE DETAIL

COMPUTATIONAL CHEMISTRY

Country

Korea, South

Host Institution

Korea University

Program(s)

Korea University

UCEAP Course Level

Upper Division

UCEAP Subject Area(s)

Chemistry

UCEAP Course Number

103

UCEAP Course Suffix**UCEAP Official Title**

COMPUTATIONAL CHEMISTRY

UCEAP Transcript Title

COMP CHEMISTRY

UCEAP Quarter Units

4.50

UCEAP Semester Units

3.00

Course Description

Due to the constantly increasing computational power and the rise of density functional theory (DFT) and artificial intelligence (AI), computational approaches to chemistry are booming. We are now able to simulate almost every chemical process at multiple times and size scales and discuss macroscopic thermodynamic and kinetic trends from a quantum chemical perspective. This course enters this exciting field by first introducing computational chemistry, then learning about DFT and how to use it to calculate reaction energies, MO diagrams, kinetic barriers, etc., run molecular dynamics simulations, and basic machine learning.

Recommended Prerequisite: The lecture requires basic physical chemistry and mathematics lecture background. Quantum chemistry background will make things easier to understand, but it is not a prerequisite. The course teaches programming and revisits quantum chemistry.

Language(s) of Instruction

English

Host Institution Course Number

CHEM452

Host Institution Course Title

COMPUTATIONAL CHEMISTRY

Host Institution Course Details

<https://infodepot.korea.ac.kr/lecture1/lecsubjectPlanView.jsp?year=2023&term=2R...>

Host Institution Campus

Host Institution Faculty

Host Institution Degree

Host Institution Department

Chemistry

Course Last Reviewed

2023-2024

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