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 Campus

Host Institution Faculty

Host Institution Degree

Host Institution Department
Chemistry

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