

COURSE DETAIL

QUANTUM CHEMISTRY AND MOLECULAR THERMODYNAMICS

Country

Singapore

Host Institution

National University of Singapore

Program(s)

National University of Singapore

UCEAP Course Level

Upper Division

UCEAP Subject Area(s)

Chemistry

UCEAP Course Number

131

UCEAP Course Suffix**UCEAP Official Title**

QUANTUM CHEMISTRY AND MOLECULAR THERMODYNAMICS

UCEAP Transcript Title

QUANTUM CHEMISTRY

UCEAP Quarter Units

6.00

UCEAP Semester Units

4.00

Course Description

This course on quantum chemistry and thermodynamics covers a wide range of topics. The first half of the course concerning quantum chemistry covers classical to quantum mechanics, (time-independent) Schrödinger equation, Quantum Mechanical Postulates, application of QM to simple systems and problems, commuting and non-commuting operators, QM model for rotation and vibration of molecules; Harmonic oscillator and rigid rotor models, the hydrogen atom: radial and angular solutions of the Schrödinger equation, multi-electronic atoms: spectroscopic terms, multiplets; Pauli Exclusion Principle, Spin-orbit coupling, chemical bonding on the example of H₂ molecule, molecular symmetry and elements of group symmetry, SALCs, Hartree-Fock and DFT methods, Roothaan equations for closed shell systems, and computational chemistry: an overview of the current status. The second half of the course (statistical thermodynamics) covers the following topics: statistical mechanics, probability, Boltzmann Distribution, ensembles and molecular partition functions, statistical thermodynamics, partition functions for non-interacting bi-atomic molecules, partition functions for polyatomic molecules, and molecular interactions.

Language(s) of Instruction

English

Host Institution Course Number

CM3231

Host Institution Course Title

QUANTUM CHEMISTRY & MOLECULAR THERMODYNAMICS

Host Institution Course Details

Host Institution Campus

Host Institution Faculty

Host Institution Degree

Host Institution Department

Chemistry

Course Last Reviewed

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