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 AND MOLECULAR THERMODYNAMICS

Host Institution Campus

Host Institution Faculty

Host Institution Degree

Host Institution Department
Chemistry

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