Nanyang Technological University
Division of Chemistry and Biological Chemistry

Academic Year	AY20/21	**Semester**	1
Course Coordinators	Tan Howe Siang & Loh Zhi Heng		
Course Code	CM4041		
Course Title	Quantum Chemistry and Statistical Thermodynamics		
Pre-requisites	CM3041 or by permission		
No of AUs	3		
Contact Hours	3 hours per week		
Proposal Date	6 January 2020		

Course Aims

The first part of the course aims to reinforce students with the basic concepts and applications of Quantum mechanics to various molecular, chemical and spectroscopic applications. You will learn how to use approximation methods to help solve QM problems. You will learn the basic concepts and applications of time dependent Quantum mechanics to problems in molecular, chemical and spectroscopic problems.

The second part of the course aims to introduce the principles of statistical thermodynamics. You will understand how macroscopic thermodynamic properties of molecular systems can be derived from microscopic quantum mechanical properties by applying statistical thermodynamics.

Intended Learning Outcomes (ILO)

Upon successful completion of this course, you should be able to:

1. Recognize, interpret and apply the basic concepts of Quantum Mechanics (QM) including superposition, outcomes of measurements, & uncertainty principle and the noncommutability of operators.
2. Use basis sets, complex vector space, bra-ket notation and matrices to formulate and solve QM problems
3. Explain, identify and apply the main concepts of approximation techniques in time independent QM, including Perturbation theory and the Variational method; Explain and identify basic molecular orbital theory by the application of the Rayleigh-Ritz method
4. Explain, identify and apply the main concepts of time-dependent QM; apply perturbation theory to solve time-dependent QM problems; Explain and identify basic phenomena of light-matter interaction (spectroscopy) by time-dependent QM
5. Explain the concept of statistical distribution functions and their occurrence in macroscopic systems with 10^{23} particles; compute the various parameters that characterize distribution functions
6. Describe the Boltzmann distribution and use it to calculate the relative populations of different eigenstates of a molecule; describe the molecular partition function and extend it to the ensemble partition for both distinguishable and indistinguishable particles
7. Formulate partition functions for the translational, rotational, vibrational, and electronic degrees of freedom of a molecule in the gas phase; derive the Maxwell-Boltzmann distribution; explain the role of nuclear spin statistics in the calculation of the rotational partition function

8. Employ molecular partition functions to compute various thermodynamic quantities, including chemical equilibrium constants; apply the transition state theory to calculate reaction rate constants

Course Content

The course can be divided into two parts:

Part 1: Quantum Mechanics in Chemistry

Brief review of basic concepts in Quantum Mechanics (QM). Use examples of simple systems to illustrate and reinforce the basic concepts

Introduction to the use of basis sets, complex vector space and matrices to formulate questions in QM.

Introduction to main methods of approximation in time independent QM, including 1) Perturbation theory and 2) Variational theorem and Rayleigh-Ritz method: applications to explain molecular orbital theory

Introduction to time dependent QM. Apply perturbation theory to solve Time dependent QM problems

Applications to Light-matter interaction (spectroscopy) in simple systems

Part 2: Statistical Thermodynamics

Brief review of probability and statistics

Microstates, configurations, Boltzmann distribution law, the molecular partition function, Ergodic hypothesis and the a priori postulate of statistical thermodynamics

Ensemble partition function, derivation of thermodynamic parameters – internal energy, Gibbs free energy, Helmholtz free energy, enthalpy, entropy, pressure, chemical potential – from partition functions

Translational partition function, Maxwell-Boltzmann Distribution Law

Partition functions for the electronic degree of freedom, atomic and molecular term symbols

Partition functions for vibrational and rotational degrees of freedom, nuclear spin statistics

Application to the calculation of chemical equilibrium constant and chemical reaction rate constants, transition-state theory

Assessment (includes both continuous and summative assessment)

Component	Course ILO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/ Individual	Assessment rubrics

1. Homework	1, 2, 3, 4, 5, 6, 7, 8	Competence, Creativity	20%	Individual	Point-based marking (not rubrics based)
2. Midterm Test 1	1, 2, 3, 4	Competence, Creativity	10%	Individual	Point-based marking (not rubrics based)
3. Midterm Test 2	5, 6, 7, 8	Competence, Creativity	10%	Individual	Point-based marking (not rubrics based)
4. Examination	1, 2, 3, 4, 5, 6, 7, 8	Competence, Creativity	60%	Individual	Point-based marking (not rubrics based)
Total			100%		

Formative feedback

You will be given feedback in four ways:

1. By working through examples provided during lectures
2. By response to postings on the course discussion board
3. By attending consultation hours
4. By studying the comments provided by the instructors after the grading of homework and midterm tests

Learning and Teaching approach

Lectures	Face-to-face lectures will be employed to enable you to interact directly with the instructor.

Reading and References

Recommended textbook: Physical Chemistry, 10th Ed. (2014), by Peter Atkins and Julio de Paula, Oxford University Press; ISBN-13: 978-0-19-969740-3

Recommended textbook: Elements of Statistical Thermodynamics, 2nd Ed. (2006), by Leonard K. Nash, Dover Publications; ISBN-10: 0-486-44978-5

Course Policies and Student Responsibilities

(1) General

You are expected to read the lecture materials prior to the lecture session in question. This will help you to learn much more efficiently as you will already have an impression on the topics to be covered. You should also read the textbook and to attempt the exercises provided in the problem sets.

(2) Absenteeism

If you miss a lecture, you are expected to make up for the lost learning activities. If you miss the mid-term test with approval, you will either be offered a make-up test or grading based upon the final exam score.

Academic Integrity

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values.

As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the academic integrity website for more information. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Course Instructors

Instructor	Office Location	Phone	Email
Tan Howe Siang	SPMS-CBC-03-06	6316 2987	howesiang@ntu.edu.sg
Loh Zhi Heng	SPMS-CBC-01-19A	6592 1655	zhiheng@ntu.edu.sg

Planned Weekly Schedule

Week	Topic	Course ILO	Readings/Activities
1	Review of basic concepts in Quantum Mechanics (QM): superposition, outcomes of measurements, & uncertainty principle and the noncommutability of operators. Use examples of simple systems to illustrate and reinforce the basic concepts.	1	Lecture, problem set
2	Introduction to the use of basis sets, complex vector space and matrices to formulate questions in QM.	2	Lecture, problem set
3	Introduction to main methods of approximation in time independent QM; Perturbation theory	3	Lecture, problem set
4	Variational theorem and Rayleigh-Ritz method. Applications to explain molecular orbital theory	3	Lecture, midterm test
5	Revision, exercises and midterms	1,2,3	Lecture, midterm test
6	Time dependent QM. Perturbation theory methods to solve Time dependent QM	4	Lecture, problem set

7	Applications to selected problems in light-matter interaction and spectroscopy	4	Lecture, problem set
8	Brief review of probability and statistics, introduction to microstates and configurations, derivation of the Boltzmann Distribution Law and the molecular partition function	5	Lecture, problem set
9	Extension of the molecular partition function to the ensemble partition function, application of partition functions to calculate thermodynamic quantities	6	Lecture, problem set
10	Introduction to the translational partition function and derivation of the Maxwell-Boltzmann Distribution Law	7	Lecture, problem set
11	Introduction to the electronic partition function, and atomic and molecular term symbols, midterm test 2	7	Lecture, midterm test
12	Introduction to the vibrational and rotational partition functions, nuclear spin statistics	7	Lecture, problem set
13	Application of partition functions to calculate chemical equilibrium constants and reaction rate constants	8	Lecture, problem set

CBC Programme Learning Outcome

The Division of Chemistry and Biological Chemistry (CBC) offers an undergraduate degree major in Chemistry that satisfies the American Chemical Society (ACS) curricular guidelines and equips students with knowledge relevant to the industry. Graduates of the Division of Chemistry and Biological Chemistry should have the following key attributes:

1. Competence

Graduates should be well-versed in the foundational and advanced concepts of chemical science, be able to evaluate chemistry-related information critically and independently, and be able to use complex reasoning to solve emergent chemical problems.

2. Creativity

Graduates should be able to synthesize and integrate multiple ideas across the curriculum, and propose innovative solutions to emergent chemistry-related problems based on their training in chemistry.

3. Communication

Graduates should be able to demonstrate clarity of thought, independent thinking, and sound scientific analysis and reasoning through written and oral reports to audiences with varying technical backgrounds. They should also be able to effectively engage other professional chemists in collaborative endeavours.

4. Character

Graduates should be able to act in responsible ways and uphold the high ethical standards that the society expects of professional chemists.

5. Civic-mindedness

Graduates should be aware of the impact of chemistry on society, and how chemistry can be applied to benefit mankind. They should also be aware of and uphold the best chemical safety practices.