Nanyang Technological University
Division of Chemistry and Biological Chemistry

Academic Year	AY20/21	**Semester**	1
Course Coordinators	Loh Zhi Heng & Edwin Yeow		
Course Code	CM3041		
Course Title	Physical and Biophysical Chemistry 2		
Pre-requisites	CM2041 or by permission		
No of AUs	3		
Contact Hours	3 hours per week		
Proposal Date	20 February 2020		

Course Aims

This course aims to introduce the principles of quantum mechanics and molecular spectroscopy, as applied to chemistry. You will understand and appreciate how quantum mechanics describes the behavior of atoms and molecules. You will understand how quantum mechanics forms the framework for interpreting molecular spectra, and the application of the equations derived from quantum mechanics to understand rotational, vibrational and electronic spectroscopy. You will also be introduced to the photophysics and photochemistry of light-excited molecules.

Intended Learning Outcomes (ILO)

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

1. Describe the various phenomena that indicate the breakdown of classical physics, the postulates of quantum mechanics, and the properties of wave functions
2. Perform mathematical manipulations with eigenfunctions and eigenvalues, expectation values, the Schrödinger equation, and employ operators to compute the expectation values of various observables
3. Solve the Schrödinger equation for the one-dimensional particle-in-a-box model and employ the solutions to compute expectation values and probabilities; extend the one-dimensional solution to the case of multi-dimensional problems; explain quantum tunneling and describe the quantitative behavior of wave functions in a tunneling barrier
4. Identify the various terms that appear in the Hamiltonians of the harmonic oscillator, two- and three-dimensional rigid rotors, and the hydrogen atom; recognize the eigenfunctions and give the eigenenergies; employ the eigenfunctions to calculate expectation values and probabilities
5. Describe electron spin, the Pauli exclusion principle, and the treatment of many-electron atoms by the orbital approximation
6. Describe the electronic structure of diatomic and simple polyatomic molecules by using valence-bond theory, molecular orbital theory, and the Hückel approximation
7. Describe various physical phenomena in chemistry by using quantum mechanics; identify an appropriate Hamiltonian to apply to a given quantum mechanical system and to obtain insight into the physical properties of the system
8. Describe, explain and apply the concepts related to rotational spectroscopy including energy levels of rigid and non-rigid rotors, selection rules, position and intensity of peaks.
9. Describe, explain and apply the concepts related to vibrational spectroscopy including degrees of freedom, vibration in diatomic molecule, harmonic and anharmonic oscillator, selection rules and rovibrational spectroscopy.

10. Describe, explain and apply the concept related to the Franck-Condon Principle on electronic spectroscopy.
11. Describe, explain and apply the concepts related to photophysics and photochemistry including Jablonski diagram, radiative and non-radiative decay pathways, Kasha's rule, emission quantum yields and lifetimes, quantum yield of photochemical reactions and photochemical rate equations.
12. Describe, explain and apply concepts related to other topics related to spectroscopy and photochemistry. This may vary from year to year.

Course Content

Blackbody radiation, the photoelectric effect, wave-particle duality, the Heisenberg uncertainty principle, and the need for a new theory: quantum mechanics

Eigenvalues and eigenfunctions, operators, observables, the Schrödinger equation and the Hamiltonian, expectation values, the Born interpretation, the postulates of quantum mechanics

Analytical solution of the Schrödinger equation for the one-dimensional particle in a box, eigenfunctions, eigenenergies, expectation values of position and momentum, quantum tunneling

Classical harmonic oscillator, the harmonic approximation, the Hamiltonian for the quantum mechanical harmonic oscillator, features of the eigenfunctions and the eigenenergies

Rigid rotors, angular momentum, features of the eigenfunctions and the eigenenergies of two- and three-dimensional rigid rotors, shapes of spherical harmonics, 3D visualization of angular momentum vectors

Hydrogen atom and its Hamiltonian, the radial wave function and its properties, radial distribution function, eigenenergies of the hydrogen atom

Electron spin, the orbital approximation for multielectron atoms, and the Pauli exclusion principle

Molecular structure as described by valence-bond theory, molecular orbital theory, and the Hückel approximation

Rotational spectroscopy, energy levels of rigid and non-rigid rotors, selection rules, position and intensity of peaks

Vibrational spectroscopy, degrees of freedom, vibration in diatomic molecule, harmonic and anharmonic oscillator, selection rules and rovibrational spectroscopy

Electronic spectroscopy and Franck-Condon Principle

Photophysics and photochemistry, Jablonski diagram, radiative and non-radiative decay pathways, Kasha's rule, emission quantum yields and lifetimes, quantum yield of photochemical reactions and photochemical rate equations.

Other topics related to spectroscopy and photochemistry. This may vary from year to year.

Assessment (includes both continuous and summative assessment)

Component	Course ILO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/ Individual	Assessment rubrics
1. Continuous assessment/ weekly assignments	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11 and 12	Competence, Creativity	15%	Individual	Point-based marking (not rubrics based)

2. Midterm Test	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11 and 12	Competence, Creativity	25%	Individual	Point-based marking (not rubrics based)
3. Examination	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11 and 12	Competence, Creativity	60%	Individual	Point-based marking (not rubrics based)
Total			100%		

Formative feedback

You will be given feedback in three 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 the midterm

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, 3rd Ed. (2013), by Thomas Engel and Philip Reid, Pearson; ISBN-13: 978-1-292-02224-6

Recommended reference textbooks:

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

Physical Chemistry, 2nd Ed. (2015), by David W. Ball, Cengage Learning; ISBN-13: 978-1-133-95843-7

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
Loh Zhi Heng	SPMS-CBC-01-19A	6592 1655	zhiheng@ntu.edu.sg
Edwin Yeow	SPMS-CBC-03-04	6316 8759	edwinyeow@ntu.edu.sg

Planned Weekly Schedule

Week	Topic	Course ILO	Readings/Activities
1	Motivation for the need for quantum mechanics, mathematical manipulations in quantum mechanics, and postulates of quantum mechanics	1, 2	Lecture, homework assignment
2	Particle-in-a box from 1-D to 3-D, quantum tunneling	3	Lecture, homework assignment
3	Harmonic oscillator	4	Lecture, homework assignment
4	Two- and three-dimensional rigid rotor	4	Lecture, homework assignment
5	Hydrogen atom	4	Lecture, homework assignment
6	Multielectron atoms	5	Lecture, homework assignment
7	Electronic structure of molecules and review	6, 7	Lecture, homework assignment
8	Introduction to spectroscopy and rotational spectroscopy	8	Lecture, homework assignment
9	Rotational spectroscopy and vibrational spectroscopy	8, 9	Lecture, homework assignment
10	Vibrational and rovibrational spectroscopy	9	Lecture, homework assignment
11	Midterm	TBA in class	Lecture, assessment
12	Review of midterm, electronic spectroscopy and photophysics	10, 11	Lecture, homework assignment

13	Photochemistry	11, 12	Lecture, homework assignment

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.