Annexe A: New/Revised Course Content in OBTL+ Format

Course Overview

Expected Implementation in Academic Year	AY2025-2026
Semester/Trimester/Others (specify approx. Start/End date)	Semester 1 Semester 2
Course Author * Faculty proposing/revising the course	Tan Howe Siang, Edwin Yeow
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Course Title	Physical and Biophysical Chemistry 2
Course Code	CM3041
Academic Units	3
Contact Hours	39
Research Experience Components	Not Applicable

Course Requisites (if applicable)

Pre-requisites	CM2041 or by permission
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

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.

Course's Intended Learning Outcomes (ILOs)

Upon the successful completion of this course, you (student) would be able to:

ILO 1	Describe the various phenomena that indicate the breakdown of classical physics, the postulates of quantum mechanics, and the properties of wave functions
ILO 2	Perform mathematical manipulations with eigenfunctions and eigenvalues, expectation values, the Schrödinger equation, and employ operators to compute the expectation values of various observables
ILO 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
ILO 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
ILO 5	Describe electron spin, the Pauli exclusion principle, and the treatment of many-electron atoms by the orbital approximation
ILO 6	Describe the electronic structure of diatomic and simple polyatomic molecules by using valence-bond theory, molecular orbital theory, and the Hückel approximation
ILO 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
ILO 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
ILO 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
ILO 10	Describe, explain and apply the concept related to the Franck-Condon Principle on electronic spectroscopy
ILO 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
ILO 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.

Reading and References (if applicable)

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

Planned Schedule

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	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

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
11	Midterm 2	TBA in class			Lecture, assignment
12	Review of midterm, electronic spectroscopy and photophysics	10,11			Lecture, homework assignment
13	Photochemistry	11,12			Lecture, homework assignment

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Lectures	Face-to-face lectures will be employed to enable you to interact directly with the instructor.

Assessment Structure

Assessment Components (includes both continuous and summative assessment)

No.	Component	ILO	Related PLO or Accreditation	Weightage	Description of Assessment Component	Team/Individual	Rubrics	Level of Understanding
1	Continuous Assessment (CA): Assignment(Homework)	1-12	Competence, Creativity	10	Online quizzes to assess understanding of the teaching materials. Accessible anytime during the assessment window.	Individual	Holistic	Multistructural
2	Continuous Assessment (CA): Class Participation()	1-12	Competence, Creativity	5	In-class quizzes delivered via an online platform (e.g., Wooclap) to assess understanding of the teaching materials.	Individual	Holistic	Multistructural
3	Continuous Assessment (CA): Test/Quiz(Midterm I)	1-7	Competence, Creativity	12.5		Individual	Analytic	Multistructural
4	Continuous Assessment (CA): Test/Quiz(Midterm II)	8-9	Competence, Creativity	12.5		Individual	Analytic	Multistructural
5	Summative Assessment (EXAM): Final exam()	1-12	Competence, Creativity	60		Individual	Analytic	Multistructural

Description of Assessment Components (if applicable)

Point-based marking (not rubrics based)

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

NTU Graduate Attributes/Competency Mapping

This course intends to develop the following graduate attributes and competencies (maximum 5 most relevant)

Attributes/Competency	Level
Creative Thinking	Intermediate
Problem Solving	Intermediate
Critical Thinking	Intermediate

Course Policy

Policy (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. On the use of technological tools (such as Generative AI tools), different courses / assignments have different intended learning outcomes. Students should refer to the specific assignment instructions on their use and requirements and/or consult your instructors on how you can use these tools to help your learning. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

Policy (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.

Policy (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.

Policy (Others, if applicable)

Diversity and Inclusion Policy
Integrating a diverse set of experiences is important for a more comprehensive understanding of science and engineering. It is our goal to create an inclusive and collaborative learning environment that supports a diversity of perspectives and learning experiences. That honours your identities; including ethnicity, gender, socioeconomic status, sexual orientation, religion or ability.
To help accomplish this:
• If you are neuroatypical or neurodiverse, have dyslexia or ADHD (for example), or have a social anxiety disorder or social phobia;
• If you feel your performance in the course is being impacted by your experiences outside of class;
• If something was said in the course (by anyone, including instructor/supervisor) that made you uncomfortable.
Please e-mail to your Associate Chair (Students & Continuing Education) at ac-cceb-stud@ntu.edu.sg about how we can help facilitate your learning experience.
As a participant in course discussions you should also strive to honour the diversity of your classmates. You can do this by; using preferred pronouns and names; being respectful of others opinions and actively making sure all voices are being heard; and refraining from the use of derogatory or demeaning speech or actions.
All members of the course are expected to strictly adhere to the student code of conduct (https://www.ntu.edu.sg/life-at-ntu/student-life/student-conduct). If you witness something that goes against this or have any other concerns, please speak to your instructors or a faculty member.

Last Updated Date: 19-11-2025 10:11:20

Last Updated By: Natasha Bhatia (Dr)