

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

Course Overview

Expected Implementation in Academic Year (New format)	AY2026-2027
Semester/Trimester/Others (specify approx. Start/End date)	Semester 2
Course Author * Faculty proposing/revising the course	Lu Yunpeng
Course Author Email	yplu@ntu.edu.sg
Course Title	MOLECULAR MODELLING:PRINCIPLES & APPLICATIONS
Course Code	CM4043
Academic Units	3
Contact Hours	39
Research Experience Components	Not Applicable

Course Requisites (if applicable)

Pre-requisites	CM3041, or CH2108 & CH2123, or by permission
Co-requisites	
Pre-requisite to	
Mutually exclusive to	
Replacement course to	
Remarks (if any)	

Course Aims

This course aims to equip undergraduate students with the theoretical foundation and practical skills necessary to independently design, execute, and interpret computational chemistry investigations using modern electronic structure methods. Building upon introductory principles, the course provides in-depth training in the ab initio and density functional theory workflows employed in contemporary research, spanning geometry optimisation, transition-state searching, solvation modelling, and the prediction of spectroscopic and thermochemical observables. Students will develop the competency to apply computational tools—particularly Gaussian 16—to elucidate reaction mechanisms, assign spectral data, and evaluate molecular properties, thereby enabling them to bridge experiment and theory effectively in academic and industrial research settings.

Course's Intended Learning Outcomes (ILOs)

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

ILO 1	Design, execute, and validate computational chemistry experiments using Gaussian 16, including input-file preparation, potential energy surface exploration, and output analysis.
ILO 2	Select and justify appropriate electronic structure methods, basis sets, and effective core potentials for a given chemical problem, while critically evaluating computational results reported in the literature.
ILO 3	Interpret molecular orbitals, electron density, electrostatic potential maps, partial charges, and Fukui functions to predict and explain chemical reactivity and molecular properties.
ILO 4	Perform conformational analysis and relaxed potential energy scans to identify stable conformers, compare relative energies, and analyse intramolecular interactions.
ILO 5	Compute and interpret vibrational frequencies and thermochemical data, including zero-point energies, enthalpies, entropies, and Gibbs free energies, and simulate/analyse IR spectra.
ILO 6	Locate and validate transition states and reaction intermediates, and construct reaction energy profiles to elucidate organic and inorganic reaction mechanisms.
ILO 7	Apply implicit and explicit solvation models to assess solvent effects on molecular structure, energetics, and spectroscopic observables.
ILO 8	Calculate redox potentials and electrochemical properties from first principles, and relate computed values to experimental electrochemical data.
ILO 9	Apply hybrid QM/MM methods such as ONIOM and Born–Oppenheimer molecular dynamics (BOMD) to model complex chemical systems and reaction dynamics.
ILO 10	Model excited states and photochemical processes, including conical intersections, and interpret UV-vis/ECD spectra to propose photochemical mechanisms.

Course Content

1. First Contact: Input Files, the Potential Energy Surface, and Your First Calculation
2. Choosing the Right Tool: Methods, Basis Sets, and Effective Core Potentials
3. Reading Chemical Pictures: Orbitals, Density, ESP, Partial Charges, and Fukui Functions
4. Conformational Analysis and Relaxed Potential Energy Scans
5. Vibrations, Thermochemistry, and IR Spectra
6. Transition States and Reaction Mechanisms
7. Chemistry in Solution: Implicit Solvation Models
8. Redox Potentials and Electrochemistry from First Principles
9. Hybrid Modelling and Chemical Dynamics: ONIOM and BOMD
10. Photochemistry and Conical Intersections

Reading and References (if applicable)

1. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics (4th Edition)
 - **Author:** Errol G. Lewars
 - **Publisher:** Springer International Publishing
 - **Publication Year:** 2024 (4th edition)
 - **ISBN:** 978-3-031-51445-6 (Paperback); 978-3-031-51443-2 (eBook)
2. Exploring Chemical Concepts Through Theory and Computation
 - **Editor:** Shubin Liu
 - **Publisher:** Wiley-VCH Verlag GmbH
 - **Publication Year:** 2024
 - **ISBN:** 978-3-527-35248-7
3. Density-Functional Theory: A Convex Treatment
 - **Authors:** Trygve Helgaker
 - **Publisher:** John Wiley & Sons Inc.
 - **Publication Year:** 2024
 - **ISBN:** 978-1-118-94134-8

Planned Schedule

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
1	First Contact: Input Files, the Potential Energy Surface, and Your First Calculation	1	In-person	Students will be asked to develop simple Gaussian input files, run calculations and check the results	Lecture notes and slides for week 1
2	Choosing the Right Tool: Methods, Basis Sets, and Effective Core Potentials	1	In-person	Students will be asked to test about the different basis sets in calculations and compare the results for the same molecules and the same calculation methods.	Lecture notes and slides for week 2
3	Reading Chemical Pictures: Orbitals, Density, ESP, Partial Charges, and Fukui Functions	2	In-person	Students will be asked to generate the mentioned molecular representations based on the calculated wavefunctions and use them to explain chemicals' properties.	Lecture notes and slides for week 3
4	Conformational Analysis and Relaxed Potential Energy Scans	2	In-person	Students will be asked to perform potential energy surface scanning	Lecture notes and slides for week 4
5	Vibrations, Thermochemistry, and IR Spectra	3	In-person	Students will be asked to calculate molecular vibrational frequencies based on the optimal geometries. They will learn how to extract the thermochemical data for chemicals from calculations	Lecture notes and slides for week 5

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
6	Transition States and Reaction Mechanisms	3	In-person	Students will be asked to calculate transition states and reaction barrier based on ab initio calculations	Lecture notes and slides for week 6
7	Chemistry in Solution: Implicit Solvation Models	4	In-person	Students will be asked to calculate both molecular properties and reaction mechanisms in solutions.	Lecture notes and slides for week 7
8	Redox Potentials and Electrochemistry from First Principles	5	In-person	Students will be asked to calculate redox potential for electrochemistry based on thermodynamical cycle.	Lecture notes and slides for week 8
9	Hybrid Modelling and Chemical Dynamics: ONIOM and BOMD	5, 6	In-person	Students will be asked simulate molecular dynamics based on the BOMD and ONIOM methods in Gaussian 16	Lecture notes and slides for week 9
10	Photochemistry and Conical Intersections	7, 8	In-person	Students will be asked to calculate excited state chemistry based on TDDFT and other methods available in Gaussian 16	Lecture notes and slides for week 10
11	Project Presentations	9, 10	In-person	Both lecture and lab tutorial time will be used for project presentation.	
12	Project Presentations	1-4	In-person	Both lecture and lab tutorial time will be used for project presentation.	

Week or Session	Topics or Themes	ILO	Delivery Mode	Activities	Readings
13	Continuous Assessment Test	All	In-person	Both lecture and lab tutorial time will be used for midterm test	

Learning and Teaching Approach

Approach	How does this approach support you in achieving the learning outcomes?
Lectures	Present the key ideas and important steps used to solve different types of problems.
In-class Tutorials	Develop proficiency in problem solving skills. Reinforce concepts already covered in the lectures. Give an opportunity for weaker or more reserved students to clarify doubts.
Group projects	Train the class on teamwork and cohesion, as well as to boost confidence for weaker students. Develop communications skills. Students will be able to learn the importance of teamwork.

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): Project(Group Projects)	All	Competence, Communication, Civic-mindedness, Character, Creativity.	40		Individual	Holistic	Multistructural
2	Continuous Assessment (CA): Assignment(Tutorial Assignments)	All	Competence	20		Individual	Analytic	Multistructural
3	Continuous Assessment (CA): Test/Quiz(Test)	All	Competence, Creativity, Communication.	40		Individual	Analytic	Multistructural

Description of Assessment Components (if applicable)

Home assignments develop student's problem-solving skills step by step, and group projects offer the comprehensive test bed for students to demonstrate their understandings and research skills, also, they have the good chances to practice soft skills such as collaborations, task planning and critical thinking. Final examinations test on the principles introduced by this modules.

Details of the group project below:

Project: Quantum chemistry calculations to study chemical reaction mechanism

In this project, a project team is expected to read and understand a short scientific introduction about certain organic chemical reaction and use the computational software, Gaussian, to calculate transition state and to determine the reaction heat and reaction energy barriers. They are also expected to plot molecular orbitals surfaces and other relevant graphical representations on electron densities and others to interpret the nature of chemical reaction. Students are required to submit project report (<= 15 pages) and do a presentation to introduce their project outcomes.

Formative Feedback

Feedback will be provided in email communication with students to highlight student's achievements and things to be improved after group projects.

NTU Graduate Attributes/Competency Mapping

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

Attributes/Competency	Level
Collaboration	Intermediate
Communication	Intermediate
Digital Fluency	Advanced
Self-Management	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 complete all assigned pre-class readings and activities, attend all tutorial classes punctually and take all scheduled assignments and tests by due dates. You are expected to participate in all tutorial discussions and activities.

Policy (Absenteeism)

Absence from the midterm without a valid reason will affect your overall course grade. Valid reasons include falling sick supported by a medical certificate and participation in NTU's approved activities supported by an excuse letter from the relevant bodies. There will be no make-up opportunities for CA components.

Policy (Others, if applicable)

All project assignments must be submitted on time. Failure to do so will affect your score.

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 (Undergraduate) at ac-cceb-ug@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.

Technical Skills To Be Developed

All skills to be developed for this course:

Electronic Fundamentals Application
Computational Modelling
Data analysis and reporting writing skills based on the data from the computational chemistry calculations.

Last Updated Date: 06-10-2026 14:51:59

Last Updated By: Natasha Bhatia (Dr)