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

Course Overview

The sections shown on this interface are based on the templates UG OBTL+ or PG OBTL+
If you are revising/duplicating an existing course and do not see the pre-filled contents you expect in the subsequent sections e.g. Course Aims, Intended Learning Outcomes etc. please refer to Data Transformation Status for more information.

Expected Implementation in Academic Year	AY2020-2021
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

The teaching content of this course includes two parts: 1) to learn Python programming and its applications in numerical simulations in chemical science; 2) to learn basic computational chemistry and its applications with ab initio software. Content of the first part aims to build your strength in solving chemical problems with home-made computation program. Content of the second part aims to train students to be able to study organic chemistry related problems by using computational software.

Course's Intended Learning Outcomes (ILOs)

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

ILO 1	Use Numpy package for general scientific computation
ILO 2	Use Matplotlib package for data visualization
ILO 3	Use Scipy package for specific scientific computation
ILO 4	Develop python program to solve common ordinary differential equations (ODEs) and partial differential equations in chemical sciences
ILO 5	Identify computable problems in chemistry
ILO 6	Formulate meaningful study problems that you want to explore in chemistry
ILO 7	Collect/extract computational results, visualize and perform exploratory analysis on results
ILO 8	Perform ab initio calculations to study molecular properties
ILO 9	Perform ab initio calculations to study reaction mechanism of organic chemical reaction
ILO 10	Present your analysis results and problem solution via an engaging written communication.

Course Content

Numerical simulations with Python

1. Introduction to numpy package
2. Introduction to matplotlib package
3. Introduction to Scipy package
4. Numerical applications to solve ODEs and PDEs in chemical science

Computational chemistry with ab initio software
5. General principles in computational chemistry
6. ab intio calculation methods
7. Molecule Building, Visualization, Molecule databases 8. Molecular properties based on computation
9. Thermodynamics and kinetics of organic reactions 10. Analysis of organic reaction mechanisms

Reading and References (if applicable)

1. Alan Hinchliffe (2008) Molecular Modelling for Beginners, 2nd Edition, John Wiley & Sons, ISBN: 978-0-470-51314-9

2. Hill Christian (2016) Learning Scientific Programming with Python, 1st edition. Cambridge University Press. ISBN-13: 978-1107428225

Planned Schedule

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
1	Introduction to Numpy in scientific computing, Part I, Basic	1	Study several program using numpy package		Students will be asked to develop their simple program in tutorial session
2	Introduction to Numpy in scientific computing, Part II, Intermediate	1	Study several program using numpy package		Students will be asked to develop their simple program in tutorial session.
3	Introduction to Matplotlib in data visualization, Part 1, Basic	2	Study several program using Matplotlib to plot data in 2D plane		Students will be asked to develop their simple program in tutorial session
4	Introduction to Maplotlib in data visualization, Part 2, Intermediate	2	Study several program using Matplotlib to plot data in 3D plane		Students will be asked to develop their simple program in tutorial session.
5	Introduction to scipy package in scientific computing. Part I: Basic	3	Study several program using scipy package in numerical simulation		Students will be asked to develop their simple program in tutorial session.

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
6	Introduction to scipy package in scientific computing. Part II: Intermediate	3	Study several program using scipy package in numerical simulation		Students will be asked to develop their simple program in tutorial session.
7	Numerical computation applications with Python in chemical science	4	Study several program using the above packages to solve some ODEs and PDEs in chemical science and plot the results.		Students will be asked to develop their simple program in tutorial. They will also discuss the results and the connections to chemical phenomena
8	Introduction to computational chemistry I. Basic Principles	5	Lecture notes		Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the tutorial for this topic.
9	Introduction to computational chemistry II. Different Methods in ab initio Calculations	5, 6	Lecture notes		Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the tutorial for this topic.

Week or Session	Topics or Themes	ILO	Readings	Delivery Mode	Activities
10	Introduction to computational chemistry III. Graphical Representations of Molecular Properties	7, 8	Lecture notes		Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the tutorial for this topic.
11	Introduction to computational chemistry IV. General Applications of ab intio Calculations	9, 10	Lecture notes		Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the tutorial for this topic.
12	Group Project	1-4			Both lecture and lab tutorial time will be used for project presentation.
13	Group Project	5-10			Both lecture and lab tutorial time will be used for project presentation.

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	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	Summative Assessment (EXAM): Final exam()	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 two group project below:
Project I: Quantum chemistry calculations to study chemical reactions
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.
Project II: Developing numerical calculation program to solve mathematical equations with importance in chemical science
In this project, a project team is expected to read and understand a short scientific introduction on the mathematical equations with importance in chemical science, for example, the differential kinetic equations, and develop a scientific calculation program based on python to solve a kind of equation. They will also develop computer program to plot the calculation results for analysis and presentations.

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 (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.

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