Academic Year	AY23/24	**Semester**	2
Course Coordinator	Lu Yunpeng		
Course Code	CM4043		
Course Title	Molecular Modelling: Principles and Applications		
Pre-requisites	CM3041 or (CH2108 and CH2123) by permission		
No of AUs	3		
Contact Hours	Lectures: 26 hours (2 hours per week); Laboratory: 36 hours (3 hours per week)		
Proposal Date	2 August 2023		

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.

Intended Learning Outcomes (ILO)

By the end of this course, you (as a student) would be able to:

Numerical simulations with Python

1. Use Numpy package for general scientific computation
2. Use Matplotlib package for data visualization
3. Use Scipy package for specific scientific computation
4. Develop python program to solve common ordinary differential equations (ODEs) and partial differential equations in chemical sciences

Computational chemistry with *ab initio* software

5. Identify computable problems in chemistry
6. Formulate meaningful study problems that you want to explore in chemistry
7. Collect/extract computational results, visualize and perform exploratory analysis on results.
8. Perform ab initio calculations to study molecular properties.
9. Perform ab initio calculations to study reaction mechanism of organic chemical reaction
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

Assessment (includes both continuous and summative assessment)

Component	Course ILO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/Individual	Assessment rubrics
1. Group Projects	All	Competence, Communication, Civic-mindedness, Character, Creativity.	40%	Team (20%) and Individual (20%)	Appendix 2, 3
2. Lab assignments	All	Competence	20%	Individual	Appendix 1
3. Examination	All	Competence, Creativity, Communication.	40%	Individual	Point-based marking (not rubrics based)
Total			*100%*		

Formative feedback

You will receive written and verbal feedback from the lecturer for Components 2 & 3.

You will receive summative group feedback on the group project in component 1.

Learning and Teaching approach

Approach	**How does this approach support students in**

	achieving the learning outcomes?
Lectures	Present the key ideas and important steps used to solve different types of problems.
Lab 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.

Reading and References

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
3. Jeremy Harvey (2018) *Computational Chemistry*. Cambridge University Press. ISBN-13: 978-0198755500
4. Frank Jensen (2016) *Introduction to Computational Chemistry*, 3rd edition. John Wiley & Sons, ISBN-13: 978-1118825990
5. Daan Frenkel (2023) *Understanding Molecular Simulation: From Algorithms to Applications*, 3rd edition. Associated Press, ISBN-13 : 978-0323902922

Course Policies and Student Responsibilities

(1) 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.

(2) 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.

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

Use of Generative Artificial Intelligence (GAI) such as ChatGPT is allowed in the course but students need to adhere to NTU's prevailing guideline. i.e. **Give proper citations if you use any AI tool**. Extending the practice of correctly citing references in your work under NTU's policies on citation and plagiarism, the University requires students to **(i) identify any generative AI tools used** and **(ii) declare how the tools are used in submitted work**. Please note that even with acknowledgement, copying of output generated by AI tools (in part or whole) may still be regarded as plagiarism. 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
Lu Yunpeng	CBC-06-23	65132747	yplu@ntu.edu.sg

Planned Weekly Schedule

Week	Topic	Course ILO	Readings/ Activities
1	Introduction to Numpy in scientific computing, Part I, Basic	1	Readings: Study several program using numpy package Activities: Students will be asked to develop their simple program in lab tutorials
2	Introduction to Numpy in scientific computing, Part II, Intermediate	1	Readings: Study several program using numpy package Activities: Students will be asked to develop their simple

			program in lab tutorials.
3	Introduction to Matplotlib in data visualization, Part 1, Basic	2	Readings: Study several program using Matplotlib to plot data in 2D plane Activities: Students will be asked to develop their simple program in lab tutorials.
4	Introduction to Maplotlib in data visualization, Part 2, Intermediate	2	Readings: Study several program using Matplotlib to plot data in 3D plane Activities: Students will be asked to develop their simple program in lab tutorials.
5	Introduction to scipy package in scientific computing. Part I: Basic	3	Readings: Study several program using scipy package in numerical simulation Activities: Students will be asked to develop their simple program in lab tutorials.
6	Introduction to scipy package in scientific computing. Part II: Intermediate	3	Readings: Study several program using scipy package in numerical simulation Activities: Students will be asked to develop their simple program in lab tutorials.
7	Numerical computation applications with Python in chemical science	4	Readings: Study several program using the above packages to solve some ODEs and PDEs in chemical science and plot the results. Activities: Students will be asked to develop their simple program in lab tutorials. They will

			also discuss the results and the connections to chemical phenomena
8	Introduction to computational chemistry I. Basic Principles	5	Readings: Lecture notes Activities: Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the lab tutorial for this topic.
9	Introduction to computational chemistry II. Different Methods in ab initio Calculations	5, 6	Readings: Lecture notes Activities: Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the lab tutorial for this topic.
10	Introduction to computational chemistry III. Graphical Representations of Molecular Properties	7, 8	Readings: Lecture notes Activities: Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the lab tutorial for this topic.
11	Introduction to computational chemistry IV. General Applications of ab intio Calculations	9, 10	Readings: Lecture notes Activities: Students will start learning the basic operations with Gaussian 09 and GaussView 5.0 in the lab 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.

Appendix 1: Assessment Criteria for Lab Assignments
Standards Criteria

Levels of Performance	Criteria Description
A+ (Exceptional) A (Excellent)	Provides clear, efficient, working and well-documented code; evidence of programing understanding and concern for code efficiency beyond getting correct solution. Demonstrated ability to develop multiple approaches to programming task, and understanding of their respective advantages.
A- (Very good) B+ (Good)	Provides clear, efficient, working and well-documented code; evidence of programing understanding.
B (Average) B- (Satisfactory) C+ (Marginally satisfactory)	Working but limited documentation of code.
C (Bordering unsatisfactory) C- (Unsatisfactory)	Write the code with lots of help from TA and instructor. Limited code documentation or demonstration of conceptual understand.
D (Deeply unsatisfactory) F (0-44)	Lack of demonstrated conceptual understanding. Non-functional code.

Appendix 2: Assessment Criteria for Group Project (20%)
Standards Criteria

Levels of Performance	Criteria Description

A+ (Exceptional) A (Excellent)	Provides clear and meaningful study questions; appropriate methods for data presentation, manipulating and exploration; efficient, working and well-documented code; evidence of programing understanding and concern for code efficiency beyond getting correct solution. Takes an original approach to the questions; very well structured reports with good interpretations of results; evidence of excellent ability to apply knowledge taught in the course while thinking outside the box; provides clear, efficient, working and well-documented code Clearly identifies, illustrates and critically examines implications of the project in wider context of society. Provide source acknowledgement in standard citation format. All references and citations are present and correctly written.
A- (Very good) B+ (Good)	Takes a conventional approach to the question; good interpretation of results; evidence of ability to apply knowledge taught in the course; provides clear, efficient, working and well-documented code. Describes conventional links between project and wider context of society with clear illustrations, or identifies and examines implications of the project in the wider context of society. Provides source acknowledgement in standard citation format. One or two references or citations missing or incorrectly written.
B (Average) B- (Satisfactory) C+ (Marginally satisfactory)	Takes a conventional approach to the question; limited interpretation of results; evidence of some (but not significant) ability to apply knowledge taught in the course; working but limited documentation of code. States conventional links between project and wider context of society without clear illustrations, or acknowledges obvious implications of the project on the wider context of the society. Provides minimal source acknowledgement. Some information does not contain a citation.
C (Bordering unsatisfactory) C- (Unsatisfactory)	Limited understanding of process; incorrect or miss-interpreted results; limited evidence of ability to apply knowledge taught in the course. Non-functional or limited code documentation. Makes some weak connections or missed some obvious implications of the project and the wider context of society. Many references and citations are missing. Format has technical errors or is presented in inconsistent styles.
D, F (Deeply unsatisfactory)	Inadequate in addressing the question; incorrect and/or miss-interpretation of results; lacks structure and focus, and is mostly or wholly off topic; inadequate capacity to apply knowledge taught in the course; non-functional code. OR failure to submit the report.

	Makes little to no connection between the project and the wider context of society, or missed some obvious negative implications pf the project on the wider context of society. References and citation errors detract significantly from paper. Little or no acknowledgment of sources.

Appendix 3: Assessment Criteria for Individual Contribution in Group Project (20%)

	Fail standard (0-39%)	Pass standard (40-75 %)	High standard (76-100 %)
Individual Contribution	Little contribution to the project Silent on the ideas of others Little or no interaction with group members Absent or was often late and leaving early Clueless when question on basic material/concepts	Participate meaningfully in the project Show a willingness to discuss the ideas of others Cooperate with other group members Was present for most meetings, seldom late or leaving early Lead or Facilitate discussions Demonstrate familiarity with most materials/concepts when question	Contribute significantly in the development of the project Constructively critique and build on the ideas of others Play an instrumental role in getting group members to cooperate Was present and punctual for all meetings Lead and Facilitate discussions Demonstrate a high degree of familiarity with materials/concepts when question, often with detailed elaboration.

Please assess the work of you and your colleagues by using the following criteria. We will consider your feedback in assigning the grade for the project. Please try to be as honest and fair as possible in your assessment.

5 = Excellent work; was crucial component to group's success
4 = Very strong work; contributed significantly to group
3 = Sufficient effort; contributed adequately to group
2 = Insufficient effort; met minimal standards of group
1 = Little or weak effort; was detrimental to group (Written explanation to be submitted.)

SELF Evaluation (Name: _____):
_____ Participation in developing ideas and planning project
_____ Willingness to discuss the ideas of others

_____ Cooperation with other group members
_____ Interest and enthusiasm in project
_____ Participation in leading/facilitating discussion
_____ Ease and familiarity with discussion material

PEER Evaluation (Partner 1: _____):
_____ Participation in developing ideas and planning project
_____ Willingness to discuss the ideas of others
_____ Cooperation with other group members
_____ Interest and enthusiasm in project
_____ Participation in leading/facilitating discussion
_____ Ease and familiarity with discussion material

PEER Evaluation (Partner 2: _____):
_____ Participation in developing ideas and planning project
_____ Willingness to discuss the ideas of others
_____ Cooperation with other group members
_____ Interest and enthusiasm in project
_____ Participation in leading/facilitating discussion
_____ Ease and familiarity with discussion material

PEER Evaluation (Partner 3: _____):
_____ Participation in developing ideas and planning project
_____ Willingness to discuss the ideas of others
_____ Cooperation with other group members
_____ Interest and enthusiasm in project
_____ Participation in leading/facilitating discussion
_____ Ease and familiarity with discussion material

Self-Reflection

What did you learn from the experience?

What do you think went well?

What would you have done differently, given the opportunity?

Do you have any other comments or suggestions about the project?

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.