Department of Chemistry

UNIVERSITY OF CANTERBURY
Te Whare Wānanga o Waitaha
CHRISTCHURCH NEW ZEALAND

General Course Information

# CHEM 438
# Molecular dynamics

0.125 EFTS 15 Points
First Semester 2022

**Description**
This course is about modelling the behaviour of macromolecular systems (e.g. biomacromolecules such as proteins or supramolecular assemblies such as metal-organic-framework materials), using molecular dynamics. The topics covered by this course are:

- Force fields and equations of motion
- Controlling temperature, pressure, volume within simulations
- Practical considerations when running molecular dynamics simulations
- Assessing how well simulations match experiment

**Timetable**
***Workshops:*** One hour per week. Details to be confirmed on 'My Timetable' and the Web.

Students should note that this course involves a high degree of self-guided learning. Students will be given course material and assignment instructions in advance and must come to workshops prepared with questions on the assignment material. The first workshop will be a course intro.

**Course Coordinator**
Associate Professor Deborah Crittenden, School of Physical and Chemical Sciences, BT Room 326, ext 95217 email: deborah.crittenden@canterbury.ac.nz

**Assessment**
Assignments: 3 assignments worth 100% in total, comprising a mixture of written work and oral presentations.

**Prerequisites**
P: 300-L CHEM or BCHM

**Web-based resources**
All learning resources for this course will be available via the University of Canterbury's *Learn* web site -- http://learn.canterbury.ac.nz/.

**Goal of the Course**
The goal of this course is for students to understand how molecular dynamics simulations work, how to meaningfully generate and analyse molecular dynamics data, and be able to critically assess molecular dynamics results presented in the literature.

**Learning Outcomes**

*As a student in this course I will develop the ability to:*

- *Define what is meant by the terms "force field" and "equations of motion" and describe the relationship between them in the context of performing molecular dynamics simulations*
- *Perform all of the steps of a molecular dynamics simulation for a simple model system*
- *Explain how differences in the force field affect the outcome of molecular dynamics trajectories*
- *Explain how differences in initial conditions (displacements and velocities) affect the outcome of molecular dynamics trajectories*
- *Explain how the choice of time step affects the accuracy of a simulation*
- *Recognise how these basic steps can be generalized to simulate systems of arbitrary size and complexity*
- *Describe the additional complications that arise in larger systems (e.g. controlling pressure, volume, temperature for all atoms) and how they are controlled for within molecular dynamics simulations*
- *Describe the information required to set up and initiate molecular dynamics simulations on larger systems*
- *Describe the types of data that are produced during MD simulations and how they can be meaningfully analysed*
- *Critique the scientific literature in the light of the knowledge I have gained from the above learning outcomes.*

**Transferable Skill Register**

*As a student in this course I will develop the following skills:*

- Critical analysis of the scientific literature.
- Numeracy: being able to translate equations into simulation processes
- Presentation: the ability to explain what you have learned to a scientifically literate audience
- Writing: the ability to explain yourself clearly and logically in writing.

**Summary of the Course Content**

The topics coved by this course are:

***MOLECULAR DYNAMICS FUNDAMENTALS*** **(4 workshops)**

In this part of the course, you will complete your first assignment: constructing your own molecular dynamics trajectory for an oscillating diatomic molecule and exploring how the results change if you change the input parameters.

***MOLECULAR DYNAMICS PRINCIPLES*** **(4 workshops)**

In this part of the course, you will complete your second assignment: summarizing and explaining all of the additional information required to meaningfully run and analyse molecular dynamics simulations on more realistic chemical and biochemical systems.

***MOLECULAR DYNAMICS APPLICATIONS*** **(4 workshops)**

In this part of the course, you will choose a scientific article from the literature that presents both experimental and molecular dynamics results and critically assess the match between the two, i.e. how well/appropriately the MD simulations predict and/or explain experiment.

# GENERAL INFORMATION 2022

**Chemistry Department Policy on 'Dishonest Practice'**
The University has strict guidelines regarding 'dishonest practice' and 'breach of instructions' in relation to the completion and submission of examinable material. In cases where dishonest practice is involved in tests or other work submitted for credit a department may choose to not mark such work ('Academic Integrity and Breach of Instruction Regulations').

The Department of Chemistry upholds this policy. It considers plagiarism, collusion, copying, and ghost writing to be unacceptable and dishonest practices:

- ***Plagiarism*** is the presentation of any material (text, data or figures, on any medium including computer files) from any other source without clear and adequate acknowledgement of the source.
- ***Collusion*** is the presentation of work performed in whole, or in part, in conjunction with another person or persons, but submitted as if it has been completed by the named author alone. This interpretation is not intended to discourage students from having discussions about how to approach an assigned task and incorporating general ideas that come from those discussions into their own individual submissions, but acknowledgement is necessary.
- ***Copying*** is the use of material (in any medium, including computer files) produced by another person or persons with or without their knowledge and approval. **This includes copying of the lab reports (raw data may be shared within the group if permitted or required by the experiment) - data analysis and interpretation of obtained results MUST be performed individually.**
- ***Ghost writing*** is the use of other person(s) (with, or without payment) to prepare all or part of an item of work submitted for assessment.

**Additional Information**
***Special consideration of assessment*:** If you feel that illness, injury, bereavement or any other critical extenuating circumstance beyond your control has prevented you from completing an item of assessment or affected your performance in that assessment, you may apply for special consideration. Special consideration is not available for items worth less than 10% of the course. Applications for special consideration should be made **within five days** of the due date for the work or examination. In the case of illness or injury, medical consultation should normally have taken place shortly before, or within 24 hours after, the due date for the required work or the date of the test or examination. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. ***You have the right to appeal any decision.***

***Extensions of deadlines:*** Where an extension may be granted for an assessment item, this will be decided by application to the course co-ordinator.

***Late withdrawal from the course***: If you are prevented by extenuating circumstances from completing the course after the final date for withdrawing from the course, you may apply for special consideration for late discontinuation. For details on special consideration, or to make an application, refer to the Examinations Office website http://www.canterbury.ac.nz/exams/. Applications must be submitted ***within five days*** of the end of the main examination period for the semester.

***Missing of tests*:** In rare cases a student will not be able to sit a test. In such cases, the student should consult with the course co-ordinator to arrange alternative procedures. **This must be done well in advance of the set date for the test.**

***Submission of reports and assignments*: Reports (including lab reports) and assignments should be handed in on time.** Extensions will be granted only in exceptional circumstances (such as illness or bereavement). If an extension is required, as early as possible you should request it from the lecturer concerned.
*Note:* If you do not submit an assignment for assessment, you will be allotted zero marks, which will affect your final result. You should ensure that you pick up marked assignments and keep them until the end of the course as evidence that the work was completed and marked in the case that either is disputed. To guard against accidental loss, it would be prudent to keep photocopies or electronic copies of anything submitted.

***Late Work:*** Late work should be accompanied by a detailed explanation of why the work is late. The work will be marked and **10% of the total marks will be subtracted for *each day* the work is late**. Days late include weekends and holidays.

***Marks and Grades:*** The following numbers should be considered as a guide to the expected grades under normal circumstances. The School reserves the right to adjust mark/grade conversions, if necessary.

***Please note that for all invigilated assessments (tests and exams) worth 33% and above, failure to obtain a mark of at least 40% will result in a final grade no higher than an R at 100 and 200 level, and a C- at 300 level.***

| **Grade:** | **A+** | **A** | **A−** | **B+** | **B** | **B−** | **C+** | **C** | **C-** | **D** | **E** |
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| **Minimum mark %:** | **90** | **85** | **80** | **75** | **70** | **65** | **60** | **55** | **50** | **40** | **0** |

***Reconsideration of Grades:*** Students should, in the first instance, speak to the course co-ordinator about their marks. If they cannot reach an agreeable solution, or have questions about their grade in a course, students should then speak to the Coordinator of 400-level studies, Dr Sarah Masters (Room 422, Beatrice Tinsley Building, phone 369 4229). Students can appeal any decision made on their final grade. You can apply at the Registry for reconsideration of the final grade within four weeks of the date of publication of final results. Be aware that there are time limits for each step of the appeals process.

***Students with Disabilities:*** Students with disabilities should speak with someone at Equity and Disability Service, phone: 369 3334 (or ext. 93334), email: eds@canterbury.ac.nz).

***Academic Advice*:** Dr Dan Foley is the coordinator of postgraduate chemistry courses. His interest is in the academic performance and well-being of all such students. Anyone experiencing problems with their chemistry courses or requiring guidance about their postgraduate studies should get in contact with Dan.

Dan Foley
Coordinator of Postgraduate Studies
School of Physical and Chemical Sciences
February 2022