PX923-7.5 Biomolecular simulation

22/23

Department
Physics
Level
Taught Postgraduate Level
Module leader
Nicholas Hine
Credit value
7.5
Module duration
5 weeks
Assessment
50% coursework, 50% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

N/A.

Module web page

Module aims

The aim of the module is to describe computational methods used in physical chemistry and their application to study the structure and dynamics of biological molecules.
A number of methods in molecular simulation, and their respective theoretical foundations, will be presented. There will be an emphasis on approaches used to probe biological phenomena and calculations of properties pertinent to biological systems.

Outline syllabus

This is an indicative module outline only to give an indication of the sort of topics that may be covered. Actual sessions held may differ.

1. Force fields for biomolecular simulation.
2. Free energy calculations. Thermodynamic integration and perturbation; potentials of mean force.

3. Advanced sampling. Biased sampling methods, replica exchange molecular dynamics. Coarse-graining for biomolecular simulation.
4. Calculated properties. Energetics, structure and dynamics; relationship to experimentally determined quantities.
5. Example applications. Drug-enzyme binding free energies and computer-aided drug design, protein structure prediction, delivery of pharmaceuticals across lipid membranes, the interface between nanomaterials and biological systems.

Learning outcomes

By the end of the module, students should be able to:

- Students will be able to describe the theoretical background and application of a selection of computational methods (including molecular dynamics, free energy calculations and techniques to study rare events) in biophysical chemistry.
- Students will have an appreciation of the advantages and disadvantages of different computational methods in the context of solving particular biological problems (e.g. protein folding, membrane transport, drug binding).
- Students will be able to evaluate the strengths and weaknesses of biomolecular simulation studies found in the literature.
- Students will be able to perform and analyse computational calculations involving biological molecules and relate them to experimental data.

Indicative reading list

● A.R. Leach, Molecular Modelling: principles and applications, Longman (1996).
● M. Tuckerman, Statistical Mechanics, Oxford Graduate Texts (2010).
● D. Frenkel & B. Smit, Understanding Molecular Simulation, From Algorithms to Applications (2001).
● A selection of papers from the recent research literature, that may change from year to year, will also be provided.

Subject specific skills

Students will be able to describe the theoretical background and application of a selection of computational methods (including molecular dynamics, free energy calculations and techniques to study rare events) in biophysical chemistry.
Students will have an appreciation of the advantages and disadvantages of different computational methods in the context of solving particular biological problems (e.g. protein folding, membrane transport, drug binding).
Students will be able to evaluate the strengths and weaknesses of biomolecular simulation studies found in the literature.
Students will be able to perform and analyse computational calculations involving biological molecules and relate them to experimental data.

Transferable skills

Biochemistry knowledge, programming, data analysis

Study

Study time

Type	Required
Lectures	5 sessions of 2 hours (13%)
Practical classes	2 sessions of 2 hours (5%)
Private study	36 hours (48%)
Assessment	25 hours (33%)
Total	75 hours

Private study description

Reading etc

Costs

No further costs have been identified for this module.

Assessment

You do not need to pass all assessment components to pass the module.

Assessment group C

	Weighting	Study time
Computational Workshop Projects 1 and 2	50%	20 hours
One piece of assessed work based on the workshops. Write up of the 2 computational workshops.		
Viva Voce Exam	50%	5 hours
Duration 15 minutes. On the core material.		

Feedback on assessment

-\tWritten feedback on assessed work.\r\n-\tVerbal discussion during viva voce exam.\r\n-\tWritten summary of viva performance.

Past exam papers for PX923

Availability

Courses

This module is Core optional for:

- Year 1 of TPXA-F344 Postgraduate Taught Modelling of Heterogeneous Systems

This module is Core option list A for:

- Year 2 of TPXA-F345 Postgraduate Taught Modelling of Heterogeneous Systems (PGDip)