CH419-15 Quantum and Atomistic Modelling

26/27

Department
Chemistry
Level
Undergraduate Level 4
Module leader
Livia Bartok-Partay
Credit value
15
Module duration
10 weeks
Assessment
20% coursework, 80% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

An introduction to atomistic modelling techniques including DFT, classical force field methods and an appreciation of how they interact with other modelling frameworks. Students will learn how to design atomistic simulations of condensed matter or molecular systems, and how to identify simulation methodologies appropriate to bridging multiple length scales, balancing accuracy vs. cost. They will gain exposure to software packages supporting interoperability between methods, e.g. the Atomic Simulation Environment. Multiscale Modelling case studies by guest lecturers will show how problems involving heterogeneous systems are tackled at multiple length & time scales.

Module web page

Module aims

To provide students with understanding and experience of atomistic modelling techniques and an appreciation of how they interact with other modelling frameworks. This will be conveyed through lectures, tutorial workshops, case studies and web pages.

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.

- Hierarchy of accuracy and different lengths- and time-scales in atomistic modelling.
- Essential statistical mechanics, sampling various ensembles using MD and MC techniques. Verlet-algorithm, thermostats, barostats, particle insertion/deletion. Calculating typical observables from simulations.
- Classical force-fields, many-body potentials, charged systems and long-range correction.
- Free-energy calculations, reaction coordinate, sampling phase equilibria.
- Single-electron quantum mechanics relevant to atomistic modelling, many-body Schrodinger equation
- The Hohenberg-Kohn and Kohn-Sham formulations of density functional theory, and their implications for accuracy and predictive power.
- Methodological choices for implementing DFT; Scaling of computational effort in DFT.

Learning outcomes

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

- Understand the context of quantum chemistry methods, density functional theory, and atomistic force-field-based modelling, and their use in a multiscale modelling context and an overview of how & why uncertainty and error can propagate between lengthscales.
- Be familiar with the common approximations and methodological choices required to implement DFT, and appreciate the widespread applications of DFT.
- Understand the ideas underlying classical force-fields and their applications.
- Have had exposure to case studies of multiscale modelling based upon atomistic calculations.
- Apply the above methods in practice.
- Have had exposure to software environments to aid interoperability between methods (eg the Atomic Simulation Environment in Python).
- Design an atomistic simulation to extract a particular property of a condensed matter or molecular system.
- Identify simulation methodologies appropriate to bridging multiple lengthscales, balancing accuracy vs cost.

Indicative reading list

Reading lists can be found in Talis

Specific reading list for the module

Subject specific skills

Understand the context of quantum chemistry methods, density functional theory, and atomistic

force-field-based modelling, and their use in a multiscale modelling context and an overview of how & why uncertainty and error can propagate between lengthscales
Be familiar with the common approximations and methodological choices required to implement DFT, and appreciate the widespread applications of DFT
Understanding of the ideas underlying classical force-fields and their applications
Exposure to case studies of multiscale modelling based upon atomistic calculations

Transferable skills

Exposure to software environments to aid interoperability between methods (eg the Atomic Simulation Environment in Python)
The ability to design a simulation to extract a particular property of a condensed matter or molecular system.
The ability to identify appropriate simulation methodologies, balancing accuracy vs cost.

Study

Teaching split

Provider	Weighting
Chemistry	50%
Physics	50%

Study time

Type	Required	Optional
Lectures	9 sessions of 2 hours (12%)	
Supervised practical classes	1 session of 3 hours (2%)	1 session of 3 hours
Private study	126 hours (84%)	
Assessment	3 hours (2%)	
Total	150 hours	

Private study description

Further reading and quantum mechanics background revision.

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 D

	Weighting	Study time	Eligible for self-certification
Assessment component			
Computational Workshops	20%	3 hours	No
Students must attend one workshop of their choice in preparation for completion of this assessment. The assessment comprises notebooks implementing programming and data analysis exercises based on atomistic simulations.			
Reassessment component is the same			
Assessment component			
Written examination	80%		No

- Students may use a calculator
- Periodic Tables
- Answerbook Pink (12 page)

Reassessment component is the same

Feedback on assessment

Written annotations to submitted computational notebooks
Cohort level feedback on written examination

Past exam papers for CH419

Availability

Courses

This module is Optional for:

- UCHA-F110 Undergraduate Master of Chemistry (with Industrial Placement)
  - Year 4 of F110 MChem Chemistry (with Industrial Placement)
  - Year 4 of F112 MChem Chemistry with Medicinal Chemistry with Industrial Placement
- Year 5 of UCHA-F107 Undergraduate Master of Chemistry (with Intercalated Year)
- UCHA-F109 Undergraduate Master of Chemistry (with International Placement)
  - Year 4 of F109 MChem Chemistry (with International Placement)
  - Year 4 of F111 MChem Chemistry with Medicinal Chemistry (with International Placement)
- UCHA-4M Undergraduate Master of Chemistry Variants
  - Year 4 of F105 Chemistry
  - Year 4 of F125 MChem Chemistry with Medicinal Chemistry
- Year 5 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)