CH413-15 Advanced Computational Chemistry

22/23

Department
Chemistry
Level
Undergraduate Level 4
Module leader
Livia Bartok-Partay
Credit value
15
Module duration
10 weeks
Assessment
25% coursework, 75% exam
Study location
University of Warwick main campus, Coventry

Description

Introductory description

N/A

Module web page

Module aims

This module is designed to develop student knowledge of, and competence in practicing, state-of-the-art methods in computational chemistry.

The module will be equally split between three members of staff in the computational chemistry section in the Department of Chemistry. In each section of the module, students will be introduced to contemporary research challenges in three distinct areas of contemporary computational chemistry:

(i) Enhanced Sampling and Machine Learning methods.
Methodological challenges: a) Enabling molecular simulations of “rare events” such as chemical reactions and phase transitions; b) Taking advantage of molecular datasets to predict the functional properties of new chemical species.

Application domain: a) Crystal nucleation and growth; b) Drug discovery

(ii) Density functional theory and materials modelling.
Methodological challenges: Achieving chemical accuracy for interactions between molecules, surfaces and between molecules and surfaces; enabling computationally efficient evaluation of structural, thermodynamic, and spectroscopic materials properties in the mesoscopic regime; Choosing the right DFT-based approach for the scientific problem in hand.

Application domain: a) Prediction of hybrid, composite and solid-state material properties, b) Heterogeneous photo- and electrocatalysis and electrochemistry.

(iii) Potential energy surfaces Methodological challenges: Description and properties of the potential energy surface; exploring the landscape: sampling techniques for finding minima, global optimisation techniques and thermodynamic properties; structure prediction. Application domain: a) clusters for catalysis b) molecular crystals for pharmaceuticals.

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In each section, learning will be supported by 4 “methodology” lectures (4 x 1hr), 1 “applications” lecture (1hr) illustrating how the three computational topics above can be used to address contemporary chemical challenges, and a computational workshop (2hrs per section) giving students a chance to see how computational chemistry methods are implemented in code examples.

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.

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Enhanced Sampling and Machine Learning methods.
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Density functional theory and materials modelling
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Potential energy surfaces

Methodological challenges: Description and properties of the potential energy surface; exploring the landscape: sampling techniques for finding minima, transition states and thermodynamic properties; structure prediction.

Application domain: a) clusters for catalysis b) molecular crystals for pharmaceuticals.

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Learning outcomes

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

- Evaluate the applicability of different computational chemistry methods in different chemical problems.
- Describe the basics of the software implementation of different computational chemistry methods.
- Discuss the contemporary challenge areas in the field of computational chemistry.
- Work with simple Python scripts of use for scientific computing.
- Apply the discussed computational chemistry methods in the context of the covered examples and workshop problems.

Indicative reading list

Enhanced sampling and machine learning:

- F. Pietrucci, “Strategies for the exploration of free energy landscapes: Unity in diversity and challenges ahead”, Reviews in Physics, 2, 32-45, (2017)
- R.J. Allen, C. Valeriani, and P.R. Ten Wolde, “Forward flux sampling for rare event simulations”, Journal of Physics: Condensed Matter, 21, 463102, (2009)
- A. Lavecchia, “Machine-learning approaches in drug discovery: methods and applications”, Drug Discovery Today, 20, 318-331, (2015)

Density Functional Theory and materials modelling:

- R. M. Dreizler, E. K. U. Gross, Density Functional Theory, Springer
- A. Gross, Theoretical Surface Science – A Microscopic Perspective, Springer
- A. E. Mattsson, P. A. Schultz, M. P. Desjarlais, T. R. Mattsson, K. Leung, Designing meaningful density functional theory calculations in materials science – a primer, Modelling Simul. Mater. Sci. Eng. 13 (2005), R1-R31
- A. J. Cohen, P. Mori-Sanchez, W. Yang, Challenges for Density Functional Theory, Chem. Rev. 112 (2012), 289-320
- P. Koskinen, V. Mäkinen, Density-functional tight-binding for beginners, Comp. Mater. Sci. 47 (2009), 237-253

Potential energy surfaces

- Energy Landscapes, D. J. Wales (Cambridge University Press).
- Introduction to Computational Chemistry, F. Jensen (Wiley).
- S. Price, Predicting crystal structures of organic compounds, Chem. Soc. Rev. 2014, 43, 2098

Research element

e.g. essay, dissertation, individual or group research, research skills activity, etc.

Subject specific skills

Problem solving
Information literacy and research skills
Digital skills and literacy

Transferable skills

Problem solving
Information literacy and research skills
Digital skills and literacy

Study

Study time

Type	Required
Lectures	15 sessions of 1 hour (10%)
Practical classes	3 sessions of 2 hours (4%)
Private study	129 hours (86%)
Total	150 hours

Private study description

Self-study: 129 hrs

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 D3

	Weighting	Study time
Computational workshop Jupyter/ipython exercises or similar	25%	
In-person Examination	75%	

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

Feedback on assessment

Feedback comments and grade on assessed work (computer workshop) provided on Moodle. Cohort level examination feedback provided via Moodle.

Past exam papers for CH413

Availability

Pre-requisites

To take this module, you must have passed:

- Any of
  - CH3F1-15 Advanced Physical Chemistry and Laboratory
  - CH3F3-30 Advanced Chemistry (Organic, Inorganic and Physical)

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 F110 MChem Chemistry (with Industrial Placement)
    - Year 4 of F109 MChem Chemistry (with International Placement)
    - Year 4 of F125 MChem Chemistry with Medicinal Chemistry
- Year 5 of UCHA-F127 Undergraduate Master of Chemistry with Medicinal Chemistry(with Intercalated Year)