UNIVERSITY of BRADFORD

Module Descriptor

Computational Crystal Engineering

Module Code:	CFS7009-B
Academic Year:	2018-19
Credit Rating:	20
School:	School of Chemistry and Biosciences
Subject Area:	Chemistry and Forensic Science (ceases 2016)
FHEQ Level:	FHEQ Level 7 (Masters)

Pre-requisites:

Co-requisites:

Contact Hours

Type	Hours
Lectures	20
Tutorials	6
Laboratory	24
Directed Study	150

Availability Periods

Occurrence	Location/Period
BDA	University of Bradford / Semester 2 (Feb - May)

Module Aims

To introduce the skills and concepts of crystal engineering and the applications of these to common problem areas. To introduce the theory of molecular mechanics and quantum mechanics as well as various aspects of applied theoretical chemistry. To be able to apply computational chemistry tools to the study of crystalline materials.

Outline Syllabus

Design concepts in organic and inorganic crystal engineering including supramolecular synthons, tectons, intermolecular interactions, co-crystallisation. The theory of crystallisation including nucleation, crystal growth applied to polymorphic, co-crystal and

salt systems. Applications of crystal engineering techniques to common problem areas such as chiral resolution, morphology modification, design of multi-component crystals for modification of physicochemical properties.
The core methods of computational chemistry, including visualisation techniques, optimisation methods, molecular mechanics, molecular dynamics and Monte Carlo modelling, perturbation calculations, conformational analysis, ab initio and semi-empirical quantum mechanics.

Use of computational chemistry software to study the structures and properties of both molecular species (organic and organometallic systems) and crystalline materials. Areas covered include solid state modelling, polymorphism, crystal morphology prediction and control, surface interactions, co-crystallisation, isostructurality, crystal structure determination / solution / prediction. The use of crystal structure databases for data mining for the design of new materials.

Module Learning Outcomes

On successful completion of this module, students will be able to...

1 Relate the principles used for modelling crystalline species

10 Apply advanced computer/IT skills

2 Detail the challenges and concepts involved in controlling crystalline phases

3 Describe the application of computational approaches to study the structures and properties of molecules solid state

4 Plan and conduct appropriate experiments in relation to experimental objectives

5 Interpret data and draw appropriate conclusions

6 Critically appraise findings and conclusions

7 Manage learning activities

8 Produce appropriate solutions to problems in context

9 Present information orally

Learning, Teaching and Assessment Strategy

The module will be delivered through a combination of lectures, workshops & practical sessions. The lectures will deliver the core theory, design concepts, computational methodology & details of common applications. The computational workshops & practical sessions will support the lecture material by allowing for the opportunity to undertake suitable computational & experimental tasks to develop the necessary practical skills. The computational sessions will include staff-led demonstration of simulation skills, detailed on-line descriptions of simulation tasks & supervision of students' simulation tasks. Practical sessions will introduce key crystallisation concepts & methods of crystal structural determination. During the module, students will undertake & report on a short research project in crystal engineering utilising computational & laboratory skills developed during the module. Topics would cover areas such as polymorph prediction, co-crystal design or modification of crystal morphology. Students will receive formative feedback on their lab notebooks & their performance in the assigned tasks, while reports on the mini research project will be formally assessed. During directed study hours, students are expected to undertake reading to consolidate & expand on the content of formal taught sessions, research & prepare for assessments and revise material from formal taught sessions, & to complete the tasks set during the workshops. The VLE will be used to provide access to online resources, lecture notes & external links to websites of interest.

Mode of Assessment

Type	Method	Description	Length	Weighting	Final Assess'
Summative	Presentation	Oral presentation on a small research project on an application of crystal engineering concepts to a selected problem		25%	No
Summative	Examination - closed book	Written examination; open questions, closed book	1.5 hours	50%	Yes
Summative	Coursework	Written report on a small research project on an application of crystal engineering concepts to a selected problem	-1000 words	25%	No

Legacy Code (if applicable)

CT-4022D

Reading List

To view Reading List, please go to **rebus:list**.