

Computational Chemistry Training Course

This course provides instruction on how to use three software packages in computational chemistry that together span the quantum and classical domains, including background on the theoretical methods. The course is aimed at researchers who may have had a light introduction to the field but now wish to pursue the subject in greater depth and gain hands-on experience in running calculations. The packages demonstrated are: GAMESS-UK (a quantum electronic structure code), ChemShell (a unix-like environment based on Tcl for coordinating QM/MM calculations), and DL-POLY (molecular dynamics code).

The expected learning outcomes are summarized below:

- An understanding of the popular methods used in computational chemistry.
- Knowledge of the key algorithms involved in a variety of widely-used computational chemistry codes.
- Experience with GAMESS-UK
- Experience with coordinating calculations using ChemShell.
- Experience with DL_POLY.

Speakers include:

- Huub Van Dam (GAMESS-UK)
- Martyn Guest (GAMESS-UK)
- Graham Fletcher (GAMESS-UK)
- Jens Thomas (CCP1 GUI)
- Paul Sherwood (ChemShell)
- Johannes Kaestner (ChemShell)
- Bill Smith (DL_POLY)
- Ilian Todorov (DL_POLY)

Equipment:

To help support these exercises we would appreciate it if attendees could bring along their own laptops. We will provide all the required software free of charge.

Schedule

Day 1 : Wednesday 11th April	
11:00 – 11:15	Introduction to the Course
11:15 – 12:00	L1 Introduction to Quantum Chemistry
12:00 – 13:00	LUNCH
13:00 – 14:00	L2 Quantum Chemistry with GAMESS-UK - Basics
14:00 – 14:30	COFFEE
14:30 – 15:00	L3 The CCP1 GUI
15:00 – 16:00	L4 ChemShell and QM/MM Modelling
16:00 – 18:00	P1 practical session (ChemShell and/or GAMESS-UK)
Day 2: Thursday 12th April	
09:30 – 10:30	L5 Hybrid QM/MM coupling options in ChemShell
10:30 – 11:00	COFFEE
11:00 – 12:00	L6 Dynamics and geometry optimization with ChemShell
12:00 – 13:00	LUNCH
13:00 – 14:30	L7 Quantum Chemistry with GAMESS-UK – Advanced
14:30 – 17:30	P2 practical session (ChemShell and/or GAMESS-UK)
Day 3: Friday 13th April	
09:45 – 10:45	L8 The DL_POLY packages
10:45 – 11:00	L9 DL_POLY SPME
11:00 – 11:30	COFFEE
11:30 – 12:00	L10 DL_POLY_3: Additional Functionality and experiences
12:00 – 13:00	LUNCH
13:00 – 16:30	P3 DL_POLY practical session