

Density Functional Methods for Experimental Spectroscopy

Monday 24 August 2009

St Edmund Hall

8:00-9:00 Breakfast (Wolfson Dinning Hall)
8:45 meet at Porters Lodge to walk to Materials Department

Hume-Rothery Lecture Theatre - Materials Department

08:50-09:10 Registration
09:10-09:15 Welcome and announcements
09:15-09:45 The Power of density-functional theory *Prof. Chris Pickard (UCL)*
09:45-10:30 The power of solid-state NMR *Dr Sharon Ashbrook (St Andrews)*
10:30-11:00 Coffee break
11:00-11:45 The Power of Vibrational Spectroscopy *Dr Timmy Ramirez-Cuesta (ISIS)*
11:45-12:30 The Power of Core-level Spectroscopy *Dr Rebecca Nicholls (Oxford)*

12:30-14:00 Lunch

Oxford University Computing Service (13 Banbury Rd)

14:00-18:00 Introduction to Crystal modelling

St Edmund Hall

19:00 Evening meal (Wolfson Dinning Hall)

Tuesday 25 August 2009

St Edmund Hall

8am-9am Breakfast (Wolfson Dinning Hall)

Hume-Rothery Lecture Theatre - Materials Department

09:15-10:15 Electronic Structure, plane-waves and pseudopotentials *Dr Phil Hasnip (York)*
10:15-10:45 Coffee break
10:45-11:45 Geometry optimization and Dynamics *Dr Jonathan Yates (Oxford)*
11:45-12:45 The reciprocal space description of electron and phonon states: DOS and dispersion *Dr Phil Hasnip (York)*

12:45-14:00 Lunch

Oxford University Computing Service (13 Banbury Rd)

2:00-3:00 Introduction to the CASTEP code *Dr Stewart Clark (Durham)*
3:00-5:30 Practical Exercises

St Edmund Hall

18:00-19:15 Poster Session (Pontigny room)
19:15 Evening meal (Wolfson Dinning Hall)

Wednesday 26 August 2009

St Edmund Hall

8am-9am Breakfast (Wolfson Dinning Hall)

Wednesday 26 August 2009 cont'd

Hume-Rothery Lecture Theatre - Materials Department

09:15-10:15 NMR methods *Dr Jonathan Yates (Oxford)*
10:15-10:45 Coffee break
10:45-11:45 Core-level spectroscopy methods *Prof. Chris Pickard (UCL)*
11:45-12:45 Vibrational spectroscopy methods *Dr Keith Refson (STFC)*

12:45-14:00 Lunch

Oxford University Computing Service (13 Banbury Rd)

14:00-18:00 Practical Exercises

St Edmund Hall

19:00 Evening meal (Wolfson Dinning Hall)

Thursday 27 August 2009

St Edmund Hall

8am-9am Breakfast (Wolfson Dinning Hall)

Hume-Rothery Lecture Theatre - Materials Department

09:15-10:15 Applications of NMR *Dr Sharon Ashbrook (St Andrews)*
10:15-10:45 Coffee break
10:45-11:45 Applications of core-level spectroscopy *Dr Rebecca Nicholls (Oxford)*
11:45-12:45 Applications in vibrational spectroscopy *Dr Timmy Ramirez-Cuesta (ISIS)*

12:45-14:00 Lunch

Oxford University Computing Service (13 Banbury Rd)

14:00-15:00 Pseudopotentials
15:00-18:00 Practical Exercises

St Edmund Hall

18:45-19:15 Drinks Reception at SEH (Old Dining Hall)
19:15 Workshop Dinner (Doctorow Hall)

Friday 28 August 2009

St Edmund Hall

8am-9am Breakfast (Wolfson Dinning Hall)

Hume-Rothery Lecture Theatre - Materials Department

09:30-10:30 Beyond DFT: exact exchange and other post-DFT methods *Dr Stewart Clark (Durham)*
10:30-11:00 Coffee break
11:00-12:00 Advanced Vibrational Spectroscopy *Dr Keith Refson (STFC)*
12:00-13:00 Future directions in electronic structure methods *Dr Peter Haynes (Imperial College)*

13:00-14:00 Lunch

Oxford University Computing Service (13 Banbury Rd)

14:00-18:00 Practical Exercises