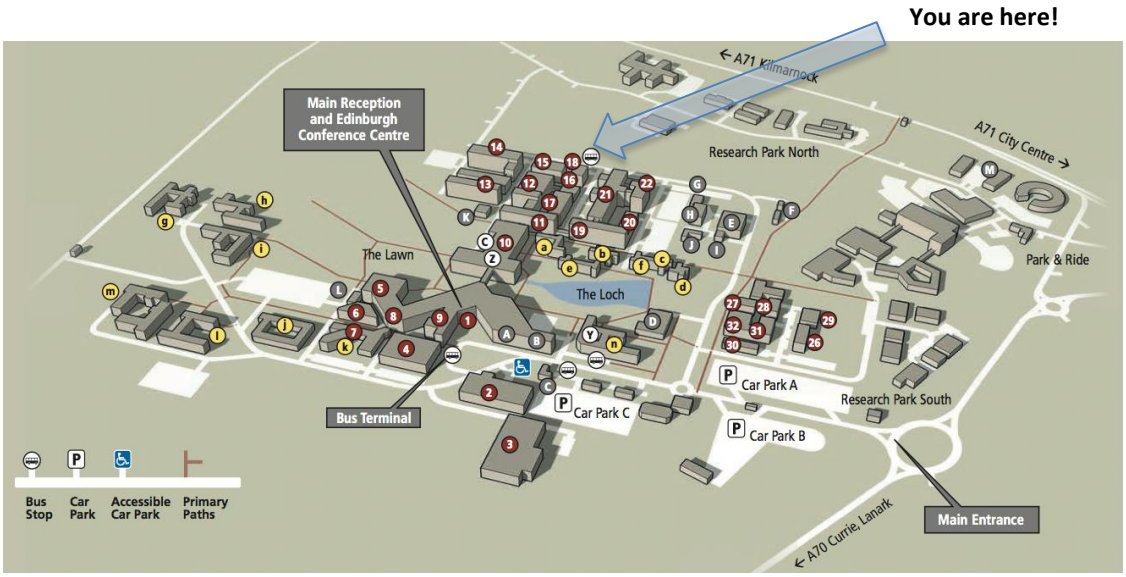
# Overview

| 9:30 – 10:20 | Registration | Postgraduate Centre |
|---|---|---|
| The registration takes place in the reception of the postgraduate centre, building 18: | | |




| 10:20 – 12:20 | Session 1 | Postgraduate Centre |
|---|---|---|
| 12:20 – 13:20 | Lunch | Earl Mountbatten Building, Room: 1.82 |
| Lunch is served in the building immediately opposite the postgraduate centre. Follow the signs! | | |

| 13:20 – 14:50 | Session 2 | Postgraduate Centre |
|---|---|---|
| 14:50 – 15:20 | Tea/Coffee | Earl Mountbatten Building, Room: 1.82 |
| 15:20 – 16:10 | Session 3 | Postgraduate Centre |
| 16:10 – 16:40 | Flash Presentations | Postgraduate Centre |
| 16:40 – 18:30 | Posters and Refreshments | Earl Mountbatten Building, Room: 1.82 and Crush Area |

# ScotCHEM 2014

## Session 1 — Chair: Prof. Martin Paterson

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|---|---|---|---|
| 10:20 | Opening Remarks<br>(Head of the Institute of Chemical Sciences) | Prof. Stuart Macgregor<br>*Heriot-Watt University* | |
| 10:30 | **PLENARY TALK:** *Mapping molecular currents: simple pictures of aromaticity and molecular conduction* | Prof. Patrick Fowler<br>*University of Sheffield* | O1 |
| 11:20 | *Computational modelling of organic semiconductors for optoelectronics* | Prof. Ian Galbraith<br>*Heriot-Watt University* | O2 |
| 11:50 | *Helical nanosystems* | Dr Ben Hourahine<br>*University of Strathclyde* | O3 |
| 12:20 | Lunch | Earl Mountbatten 1.83 | |

## Session 2 — Chair: Dr Carole Morrison

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|---|---|---|---|
| 13:20 | *Identifying trapped electronic holes at the $TiO_2$ water interface* | Dr Jun Cheng<br>*University of Aberdeen* | O4 |
| 13:50 | *Excited states and potential curves using Monte Carlo configuration interaction* | Dr Jeremy Coe<br>*Heriot-Watt University* | O5 |
| 14:10 | *Impact of ligand binding on the N-terminal MDM2 lid dynamics explored by accelerated molecular dynamics and umbrella sampling* | Dr Juan A. Bueren-Calabuig<br>*University of Edinburgh* | O6 |
| 14:30 | *Active site structure from docking and dynamics: the non-heme Fe halogenase SyrB2* | Mr Graham Rugg<br>*University of Glasgow* | O7 |
| 14:50 | Tea/Coffee | Postgraduate centre | |

## Session 3 — Chair: Dr Hans Martin Senn

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|---|---|---|---|
| 15:20 | *DFT study of a rhodium(I) σ-alkane complex: mechanism and bonding* | Dr Tobias Krämer<br>*Heriot-Watt University* | O8 |
| 15:40 | *Uncovering the mechanism of MMA production at a palladium catalyst - accounting for selectivity and reaction conditions* | Mr Luke Crawford<br>*University of St. Andrews* | O9 |
| 16:00 | *ARCHER: the UK national supercomputing service* | Dr Andrew Turner<br>*EPCC* | O10 |
| 16:10 | Flash Presentations | | |

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|---|---|---|
| F1 | **Georgios Gerogiokas** | *Biomolecular hydration thermodynamics via grid cell theory aids prediction of ligand-protein binding affinities* |
| F2 | **Nuno Almeida** | *Challenging systems for quantum chemistry: intermolecular aggregates and inorganic excited states* |
| F3 | **Greg Anderson** | Organic super-electron-donors: initiators in transition metal-free haloarene-arene coupling |
| F4 | **Divya Sharma** | *Computational analysis of benzene interaction with crystalline ice surfaces: ground and excited state investigations* |
| F5 | **Leo Holroyd** | *Mutagenic mispairing of 5-bromouracil* |
| F6 | **Peter Repiščák** | *Multi-scale computational modelling of complex molecular systems: from CuNO to polyfluorenes* |