| Poster Presentations | | |
|---|---|---|
| 1 | **Eoin Gould** | Novel trypanosomatid inhibitors inspired by nature |
| 2 | **Peter Harrison** | Towards the Biochemical and Biophysical Characterisation of Serine Palmitoyltransferase: a Human ER Multienzyme Transmembrane Complex |
| 3 | **Amanda G. Jarvis** | Artificial metalloenzymes for the selective functionalization of hydrocarbons |
| 4 | **Muhammed Ucuncu** | Bacterial Imaging and Photodynamic Therapy (PDT) Using BODIPY-Polymyxin Conjugates |
| 5 | **Sunil V. Sharma** | Living genochemetics: synchronous bio-halogenation and catalytic cross-coupling in bacterial cultures |
| 6 | **Eric Keske** | Mechanistic Studies into Rhodium Catalysed Silylation Reactions |
| 7 | **Abigail E. Watts** | SAPO STA-20: A Novel Zeotype prepared by Co-Templating Methods |
| 8 | **Chris Nottingham** | $^{13}$C-TMS-diazomethane – a versatile reagent for labelling studies |
| 9 | **Cristina Pubill-Ulldemolins** | Expanding the genochemetics toolkit with new aqueous Cross coupling methodologies |
| 10 | **Nicola L. Bell** | Uranyl reduction in a redox-active ligand |
| 11 | **David McKay** | Investigating Earth Mineral Hydration through *Ab Initio* Random Structure Searching and Solid-State NMR Spectroscopy |

EaStCHEM


University of
St Andrews

# EaStCHEM Conference for Early Career Researchers

# #ECECR2017

**Thursday 7th September 2017**
University of St Andrews
(School of Physics and Astronomy)

# EaStCHEM Conference for Early-Career Researchers 2017
# University of St Andrews
Thursday 7th September 2017

0930–1000 **Registration, Welcome Coffee and Poster Hanging**

**1000–1110 Session 1 – Academic Keynote Address** (Physics Theatre A)

**1000–1010 Welcome and Opening Remarks**
Prof. David O'Hagan

1010–1100 **KEYNOTE SPEAKER –** Dr Alyssa-Jennifer Avestro *(Durham University)*
Life in the Fast Lane: Catalysing an independent career & making it all count

1100–1110 **Comfort Break**

| **1110–1210** | **Session 2 – Early Career Researcher Presentations** | |
|---|---|---|
| | Physics Theatre A<br>*Chair: Eoin Gould* | Physics Theatre C<br>*Chair: David McKay* |
| 1110–1125 | Photoaffinity labelling identifies the target of trypanocidal bis-tetrahydropyran 1,4-triazoles<br>**Lindsay B. Tulloch** | Pump-probe simulation of $CS_2$ and CHD: time-dependent photoionization<br>**Maria Tudorovskaya** |
| 1125–1140 | Serine palmitoyltransferase protein interaction landscape and structural characterisation<br>**Van Kelly** | Ador synthesis realized by use of the hydrostatic pressure<br>**Michal Mazur** |
| 1140–1155 | Imaging intracellular drug distribution using stimulated raman scattering microscopy<br>**William J. Tipping** | Manipulation of polar order in ferroelectric 'Empty' tetragonal tungsten bronzes<br>**Jonathan Gardner** |
| 1155–1210 | Ensemble based drug design: a new paradigm in drug discovery<br>**Jordi Juárez-Jiménez** | Synthesis of magnetic polyhedral: cubes and triangular bipyramids<br>**Sergio Sanz** |

**1210–1340 Lunch, Exhibition and Poster Session** (School of Physics Common Space)

| **1340–1440** | **Session 3 – Early Career Researcher Presentations** | |
|---|---|---|
| | Physics Theatre A<br>*Chair: Tamara Kosikova* | Physics Theatre C<br>*Chair: Amanda Jarvis* |
| 1340–1355 | Mechanistic studies on nucleophilic trifluoromethylation of carbonyls with the Ruppert-Prakash reagent<br>**Thomas West** | Structure and reactivity of Cu-doped Au(111) surfaces<br>**Federico Grillo** |
| 1355–1410 | Aryloxide-facilitated catalyst turnover in α,β-unstaurated acyl ammonium catalysis<br>**Mark D. Greenhalgh** | Development of peptide-based electrochemical sensors<br>**Eva González-Fernández** |
| 1410–1425 | Studying the mechanism of C–O cleavage in lignin model compounds by ruthenium-xantphos catalysis<br>**Rebecca C. How** | *In-situ* thermal battery discharge using $NiS_2$ as a cathode material<br>**Julia Payne** |
| 1425–1440 | Towards the rational design of isoform-selective cyclophilin ligands<br>**Alessio De Simone** | Whither crystallography…<br>A view from the ground<br>**David B. Cordes** |

**1440–1510** **Afternoon Coffee** (School of Physics Common Space)

| **1510–1540** | **Session 4 – Early Career Researcher Presentations** | |
|---|---|---|
| | Physics Theatre A<br>*Chair: Mark Greenhalgh* | Physics Theatre C<br>*Chair: Rebecca How* |
| 1510–1525 | Single-molecule transmembrane supramolecular chemistry<br>**Stefan Borsley** | Molecular magnets under pressure<br>**Helen Duncan** |
| 1525–1540 | Capsules for molecular recognition and catalysis<br>**Vicente Marti-Centelles** | Difference in reactivity of two zinc binding plant metallothioneins isoforms<br>**Hasan Tanvir Imam** |

1540–1550 **Comfort Break**

**1550–1650** **Session 5 – Industry Keynote Address** (Physics Theatre A)

1550–1640 **KEYNOTE SPEAKER –** Dr Nathaniel Cain *(Afton Chemical)*
An Engineer's Career Path to Chemistry and Exploiting the Interface

**1640–1650** **Concluding Remarks and Prizegiving** (Physics Theatre A)
Neil Keddie and Amanda Jarvis

**1650–1800** **Wine Reception** (School of Physics Common Space)

**[END]**