



Marie Curie Research Training Network

Funding Scheme

MSCA-ITN-EJD - European Joint Doctorates

PARACAT

Agenda of the Winter School on Catalysis
Cardiff University, 13-17 January 2020

For more details on the PARACAT network visit:
<http://paracat.eu>



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- Monday 13th January 2020**
- 09:00 **Opening Remarks and Welcome - Student Presentations**
Damien Murphy
Venue - Beverton Lecture Theatre, Main Building, Cardiff University
- 09:15 Copper ions in zeolites with chabazite framework: an EPR and DFT characterization
Paolo Bruzzese, Leipzig University
- 09:45 Investigating the heme pocket of chlorite dismutases: biochemical and spectroscopic insights
Ilenia Serra, University of Antwerp
- 10:15 Photoactivation investigation of $\text{Cr}(\text{CO})_2\text{dppp}^+$ with UV Light by EPR for ethene oligomerization catalysis
David Fioco, Cardiff University
- 10.45 **Coffee break (room 1.67)**
- 11.00 Early EPR and chemical studies upon a new promising species of CYP450 family: the CYP116B5
Antonino Famulari, University of Zaragoza
- 11.30 EPR Characterization of Ti(III) Species in Heterogeneous Ziegler-Natta Catalysts
Leonora Podvorica, University of Turin
- 12.00 Mechanistic Investigation of Photocatalytic Reaction Processes
Andrea Guidetti, University of Antwerp
- 12.30 **Lunch (Council Chamber, Main Building)**
- 13.30 Kinetic and EPR studies of relevant peroxidases
Maruan Bracci, University of Zaragoza
- 14.00 EPR investigations on bimetallic metal organic frameworks
Kavipriya Thangavel, Leipzig University
- 14.30 The Investigation of Redox Treatment on Phillips Catalysts over Different Chromium Concentrations
Yu-Kai Liao, University of Turin
- 15.00 EPR study of Copper-tripodal complexes and their application on alcohol oxidation
Fardokht Rezayi, Cardiff University
- 15.30 **Coffee break (room 1.67)**
- 16.00 **Supervisory Board & Executive Board Meetings**
Venue - Room 0.103, Main Building, Cardiff University.
- 18.00 Board meetings end



Tuesday 14th January 2020

- 07.30 **Site visit to Diamond Light Source**
Departure from Cardiff (Main Building Car Park)
- 10.00 Introduction to Synchrotron techniques
- 10.45 Introduction to Neutron techniques
- 11.30 Tour of the Synchrotron facilities and beamlines
- 12.30 **Lunch**
- 13.00 XPS Workshop & Training Session, UK National XPS Facility
- 17.00 Departure from Harwell Research Complex

Wednesday 15th January 2020

- 0900 Tour of CCI research centre & EPR laboratories
- 12:00 **Lunch (VJ Gallery)**
Attendance at the **Cardiff Catalysis Institute Annual Conference** (15-16th Jan 2020)
Venue - Large Shandon Lecture Theatre, Main Building
- 12:45 **Opening remarks**
Duncan Wass
- 12:50 Surface molecular chemistry, a powerful tool to yield molecular supported species and calibrated nanoparticles: Applications in catalysis
Chloé Thieuleux, University of Lyon
- 13:45 Getting zeolite catalysts to play your tune
Glenn Sunley, BP Group Research
- 14:40 **Coffee and Posters (VJ Gallery)**
- 15:10 One-Pot Ammoximation of Cyclohexanone using in-situ Generated H₂O₂
Richard Lewis, CCI
- 15:35 Computational studies on the influence of support materials on the properties of Au nanoparticles
Julien Engel, CCI
- 16:05 Making light work of biological catalysis
Nigel Scrutton, University of Manchester
- 17.00 Posters with refreshments (Venue VJ Gallery)



Thursday 16th January 2020

- 08:45 Catalysis in Flow
Mimi Hii, Imperial College London
- 09:40 Catalysts for autonomous healing of composites
Richard Wingad, CCI
- 10:05 Catalysis in bacteria: whole-cell NMR to determine rate limiting step in sulphoglycolysis
Davide Zappala, CCI
- 10:30 **Coffee and Posters (VJ Gallery)**
- 10:50 Volcanos, cliffs and ways around: how to break linear scaling relationships
Nuria Lopez, Institute of Chemical Research of Catalonia
- 11:45 **The Peter Williams Memorial Lecture**
- Following electron transfer in catalytic redox processes by operando EPR “with a little help from its friends”
Angelika Brückner, Leibniz Institute for Catalysis
- 12:40 **Lunch and Posters (VJ Gallery)**
- 14.00 Free afternoon for PARACAT students
- 19.00 **Group Dinner, Cardiff Bay**



Friday 17th January 2020

Opening Remarks and Welcome - Catalysis Symposium & Ethics Workshop

Emma Richards

Venue - Small Chemistry Lecture Theatre, Main Building, Cardiff University.

- 09.00 An Emergence of SET processes in FLP Catalysis
Rebecca Melen, Cardiff University
- 09.45 Computational Databases for Prediction of Reaction Mechanisms
Natalie Fey, University of Bristol
- 10.30 **Coffee break (room 1.67)**
- 11.00 Chemistry's Ethical Landscape
Harpal Minhas, Royal Society of Chemistry
- 12.30 **Lunch (room 1.67)**
- 13.30 Iron Catalysis
Ruth Webster, University of Bath
- 14.15 Redox Active Main Group Catalysis
David Liptrot, University of Bath
- 15.00 Pulsed MW and Magnetic Fields for Sensors and Catalysis
Adrian Porch, Cardiff University
- 15.45 Electromagnetic Properties of Semiconducting Metal Oxides under External Stimulation
Daniel Slocombe, Cardiff University
- 16.30 Symposium & PARACAT Workshop close
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