

# Schedule

**Tuesday, Sept. 16<sup>th</sup>**

## Workshop - Part I

*Pfizer Lecture Theatre, Department of Chemistry  
Lensfield Road, Cambridge, CB2 1EW*

**Chair: Guido Pintacuda (CNRS/ENS Lyon, France)**

- 9.00-10:00 Registration / Visit of the Grey Group Laboratory  
Meet at Reception, Department of Chemistry
- 10.00-10.35 **Andrew Pell (University of Cambridge, UK)**  
*Introduction to Paramagnetic NMR*
- 10.35-11.10 **Tomas Vosegaard (Aarhus University, Denmark)**  
*SIMPSON Tutorial - Simulation and Visualization of Solid-State NMR Spectra*
- 11.10-11.25 Coffee break
- 11.25-12.35 **Derek Middlemiss & Ieuan Seymour (University of Warwick/Cambridge, UK)**  
*Ab Initio Modelling of Paramagnetic Shifts in Solids*
- 12.35-13.10 **Andrew Pell (University of Cambridge, UK)**  
*Practical Solid-state NMR of Paramagnetic Systems*
- 13.10-14.30 Lunch  
Todd-Hamied Room, Department of Chemistry  
(Attendees of the training workshop only)

## Conference

*McCrum Lecture Theatre, Corpus Christi College  
King's Parade, Cambridge CB2 1RH*

**Chair: Jozef Kowalewski (Stockholm University, Sweden)**

- 13.30-14.30 Registration to pNMR conference
- 14.30-14.35 **Clare Grey (University of Cambridge, UK)**  
*Welcome address*
- 14.35-15.10 **Guido Pintacuda (CNRS/ENS Lyon, France)**  
*Broadband Solid-State NMR: from Paramagnetic Metalloproteins to Battery Materials*
- 15.10-15.45 **Enrico Ravera (University of Florence, Italy)**  
*Paramagnetic NMR crystallography and DNP-enhanced NMR of Paramagnetic Crystals*
- 15.45-16.20 **Elodie Salager (CNRS Orléans, France)**  
*Space-selective and Frequency-selective NMR Spectroscopy for Lithium-ion Batteries*
- 16.20-16.50 Coffee break
- 16.50-17.25 **Ian Farnan (University of Cambridge, UK)**  
*f-electron Paramagnetic Effects in NMR Studies of Inorganic Oxides*
- 17.25-18.00 **Daniel Dawson (University of St Andrews, UK)**  
*<sup>13</sup>C NMR of Cu<sup>II</sup>-based MOFs: Acquisition, Assignment and Applications*
- 18.00-18.35 **Christophe Copéret (ETH Zürich, Switzerland)**  
*Current State of Affairs in Supported Catalysts with Paramagnetic Centres*
- 19.00-21.00 **Wine tasting offered by Cortecnet**  
Cybercafé, Department of Chemistry

Wednesday, Sept. 17<sup>th</sup>

### Conference

McCrum Lecture Theatre, Corpus Christi College  
King's Parade, Cambridge CB2 1RH

**Chair: Claudio Luchinat (CERM, University of Florence, Italy)**

- 9.00-9.35 **Tatyana Polenova (University of Delaware, USA)**  
*MAS NMR Spectroscopy of Paramagnetic Solid Materials: Rare-earth Substituted Polyoxotungstates and Vanadium-doped Microporous Titanosilicates*
- 9.35-10.10 **Jozef Lewandowski (University of Warwick, UK)**  
*Applications of Paramagnetic Effects to Study Protein Complexes by Solid-state NMR*
- 10.10-10.45 **Josef Zwanziger (Dalhousie University, Canada)**  
*Computing Materials Properties from First Principles: Towards the Right Answers for the Right Reasons*
- 10.45-11.15 Coffee break
- 11.15-11.50 **Ulla Gro Nielsen (Syddansk Universitet, Denmark)**  
*A combined Solid-state NMR and Computational Study of a Series of [Ni(II)(acac)<sub>2</sub>L<sub>2</sub>] Complexes*
- 11.50-12.25 **Rob Schurko (University of Windsor, Canada)**  
*The Basic Toolkit for Ultra-Wideline Solid-State NMR*
- 12.25-13.00 **Sylvio Indris (Karlsruhe Institut für Technologie, Germany)**  
*Li Insertion/Extraction Mechanisms and Li Mobility in Electrode Materials for Li-ion Batteries*
- 13.00-14.00 Lunch  
Dining Hall, Corpus Christi College

### Conference

McCrum Lecture Theatre, Corpus Christi College  
King's Parade, Cambridge CB2 1RH

**Chair: Juha Vaara (University of Oulu, Finland)**

- 14.00-14.35 **Brad Chmelka (University of California Santa Barbara, USA)**  
*Paramagnetic NMR and Scattering Analyses of the Structures, Compositions, and Properties of Cerium-doped Solid-state Phosphors*
- 14.35-15.10 **Gillian Goward (McMaster University, USA)**  
*<sup>6,7</sup>Li and <sup>23</sup>Na ssNMR Studies of Ion Dynamics in Cathode Materials for Lithium and Sodium Ion Batteries*
- 15.10-15.45 **Dany Carlier (ICMCB CNRS, University of Bordeaux, France)**  
*NMR Spectroscopy Combined with DFT Calculations to study Paramagnetic Materials used in Lithium (or Sodium)-ion Batteries: Towards a Better Understanding of the Chemical Bonds*
- 15.45-16.15: Coffee break
- 16.15-16.50 **Martin Kaupp (TU Berlin, Germany)**  
*Quantum-Chemical Studies of NMR Shifts of Paramagnetic Complexes: Importance of the Non-contact Terms*
- 16.50-17.25: **Philip Grandinetti (Ohio State University, USA)**  
*Measurement and Prediction of NMR Paramagnetic Shift Tensors in Solids*
- 17.30-19.30 **Poster session & drinks**  
Old and New Combination Rooms / Old court
- 19.30-21.00 **Formal dinner**  
Corpus Christi's dining Hall

Thursday, Sept. 18<sup>th</sup>

### Conference

*McCrum Lecture Theatre, Corpus Christi College  
King's Parade, Cambridge CB2 1RH*

**Chair: Clare Grey (University of Cambridge, UK)**

- 9.00-9.35 **Juan Miguel López del Amo (CIC EnergiGUNE, Spain)**  
*Solid-state NMR Characterizations of Paramagnetic and Metallic  
Compounds for Advanced Li and Na based Batteries*
- 9.35-10.10 **Scott Kroeker (University of Manitoba, Canada)**  
*Exploring NMR of Paramagnetic Solids: from Order to Disorder*
- 10.10-10.30 Coffee break

### Industrial applications of pNMR

- 10.30-11.05 **Nathan Barrow – Johnson Matthey**  
*Solid State NMR for Industrial R&D*
- 11.05-11.40 **Thomas Köster – BMW**  
*Diagnostics for Lithium ion Batteries in the Automotive Industry*
- 11.40-12.15 **Tomas Åkerud – Astra Zeneca**  
*NMR in the Pharmaceutical Industry*
- 12.15-12.20 **Clare Grey (University of Cambridge, UK)**  
*Closing remarks*

**Afternoon: pNMR mid-term Review  
(private meeting)**

Friday, Sept. 19<sup>th</sup>

**Morning: pNMR mid-term Review  
(private meeting)**

**Afternoon: pNMR Workshop - Part II**  
*Todd-Hamied Room, Department of Chemistry  
Lensfield Road, Cambridge, CB2 1EW*

- 14.00-16.00 **Guy Jones (Deputy Editor for the RSC's Inorganic Chemistry Journals)**  
*Hands-on workshop: Publishing a Scientific Paper*