SUNDAY, JULY 15, 2012

NMR crystallography and special tutorial - Z. Gan presiding	
7:00 p.m.	Opening Remarks – Rob Schurko
7:10 p.m.	**The "Smarter Approach": NMR Structure Analysis of Powdered (Organic) Solids.** *Gunther Brunklaus,* University of Muenster
7:40 p.m.	**Quantification of packing interactions in antibiotics: a combined solid-state NMR, X-ray diffraction and conputer simulation study.** *L. Mafra,* University of Aveiro
8:00 p.m.	**Recent Progress in NMR Crystallography of Zeolites and Layered Silicates.** *Darren H. Brouwer,* Redeemer University College
8:30 p.m.	**You Spin Me Right Round: Tensors and Rotations in NMR. -** Specisl Tutorial - *Leonard J. Mueller,* University of California - Riverside

MONDAY, JULY 16, 2012

Materials, Quadrupoles and First Principles Calculations, 1 - S. Ashbrook presiding	
8:20 a.m.	Opening Remarks
8:30 a.m.	**Carbon Capture, NMR, and MOF's.** *Jeffrey A Reimer,* UC Berkeley
9:00 a.m.	**Trapped Defects and Ion Mobility in Perovskites and Related Crystallographic Phases by NMR Spectroscopy.** *Frédéric Blanc,* University of Cambridge
9:20 a.m.	**A Multinuclear Solid State NMR, GIPAW DFT and MD Study of the Interstitial Conduction-Ion Species in Apatite Solid Oxide Fuel Cell Materials of the Generic Form $La_{8+x}M_{2-x}(XO_4)_6O_2$ (M = Ba, Bi, Ca, Y, Si; X = P, Si, Ge).** *John V. Hanna,* University of Warwick
9:40 a.m.	**Investigation of the structure of a new class of layered metal boronates by multinuclear solid state NMR and computational modelling.** *D. Laurencin,* Université de Montpellier 2
10:00 a.m.	*Break*
10:30 a.m.	**^{14}N Magic Angle Spinning Overtone NMR Spectroscopy.** *Luke A. O'Dell,* National Research Council Canada
11:00 a.m.	**A Study of Transition-Metal Organometallic Complexes using ^{35}Cl SSNMR, ^{35}Cl NQR and First-Principles DFT Calculations.** *Karen E. Johnston,* University of Windsor
11:20 a.m.	**^{35}Cl Solid-State NMR of Covalently-Bound Chlorine in Organic Molecules and Spectral Analysis with New Graphical Software Which Treats the Quadrupolar Interaction Exactly.** *David L. Bryce,* University of Ottawa
11:40 a.m.	**^{17}O NMR gives unprecedented insights into the structure of supported catalysts and their interaction with the silica carrier.** *L. Delevoye,* Unité de Catalyse et Chimie du Solide (UCCS - CNRS 8181)
12:00 p.m.	*Lunch (included w/registration)*
Materials, Quadrupoles and First Principles Calculations, 2 - G. Goward presiding	
1:30 p.m.	**Progress in Studying Quadrupolar Nuclei in Solids.** *Roderick E. Wasylishen,* University of Alberta
2:00 p.m.	**Hunting for Hydrogen in Wadsleyite: Multinuclear Solid-State NMR and First-Principles Calculations.** *Sharon E. Ashbrook,* University of St Andrews
2:20 p.m.	**Structure and Dynamics in Crystalline Lithium Silicides Studied by Advanced Solid State NMR Methods.** *Sven Dupke,* University of Münster
2:40 p.m.	**Application of multiple-quatum solid-state NMR experiments to the characterization of inorganic biomaterials.** *F. Fayon,* CEMHTI - CNRS
3:10 p.m.	*Break*

3:40 p.m.	**Florian A combined ^{29}Si and ^{27}Al NMR / quantum chemical study of the Al/Si ordering in Gehlenite $Ca_2Al_2SiO_7$.** *Pierre Florian*, CNRS-CEMHTI
4:00 p.m.	**A Combined First Principles and Monte Carlo Approach to the Calculation of NMR Hyperfine Shifts in Structurally Disordered, Strongly Magnetically-Coupled, or Finite-Sized Systems.** *Andrew J. Ilott*, Stony Brook University
4:20 p.m.	**Recent Advances in Oxygen-17 NMR Spectroscopy of Organic and Biological Solids.** *Gang Wu*, Queen's University
4:50 p.m.	**NMR studies of complex nuclear waste materials: phase separation, elemental partitioning and high-temperature behaviour.** *Scott Kroeker*, University of Manitoba
5:10 – 7:00 p.m.	*Conference Reception*
Posters	
7:30 - 9:30 p.m.	**Authors Present for Posters Labeled A**

TUESDAY, JULY 17, 2012

SSNMR of Biomolecules - L. Mueller Presiding	
8:30 a.m.	**Structure and Dynamics of Microtubule-Associated Protein Assemblies.** *Tatyana Polenova*, University of Delaware
9:00 a.m.	**Amyloid aggregates and large soluble protein complexes.** *Bernd Reif*, TU Muenchen
9:30 a.m.	**NMR Studies of H-Bond Acid-Base Interactions: from Model Systems to Proteins.** *Hans-Heinrich Limbach*, Freie Universitaet Berlin
10:00 a.m.	*Break*
10:30 a.m.	**Development and Application at both 9.4 and 21 T of REDOR, RFDR/SEDRA, and 2D Correlation SSNMR Approaches to Determination of Distributions of Protein: (1) Intermolecular Structures and Membrane Locations; and (2) Quantities in Whole Cells.** *David P. Weliky*, Michigan State University
11:00 a.m.	**Cross Relaxation to Sinks in CPMAS NMR of Proteins and Peptides.** *Kurt W. Zilm*, Yale University
11:20 a.m.	**Determination of the Lithium Binding Site in Inositol Monophosphatase, the Putative Target of Lithium therapy, by Magic Angle Spinning Solid State NMR.** *Amir Goldbourt*, Tel Aviv University
11:40 a.m.	**Structure and function of bacterial amyloid fibers and biofilms.** *Lynette Cegelski*, Stanford University
12:00 p.m.	*Lunch (included w/registration)*
Vaughan Symposium - Rob Schurko Presiding	
1:20 p.m.	**Introduction** - Rob Schurko
1:30 p.m.	**Solid-state NMR: Unusual conditions and using z-storage.** *Mark S. Conradi*, Washington University
2:20 p.m.	**Structure of Cysteine on Gold Nanoparticles and MAS Hardware Developments.** *Terry Gullion*, West Virginia University
3:00 p.m	*Break*
3:20 p.m.	**In-situ NMR Observation of Molecular and Ionic Processes inside Nano-Sized Pores of Activated Carbons.** *Yue Wu*, University of North Carolina
4:00 p.m.	**The Nature and Extent of Ordering in Disordered Materials: Insights from Solid-State NMR.** Jonathan F. Stebbins, Stanford University
4:40 p.m.	**High-Sensitivity Giga-Pascal NMR.** *Jürgen Haase*, University of Leipzig

5:20 – 7:20 p.m.	*SSNMR Hors D'oeuvre reception*
Posters	
7:30 – 9:30 p.m.	**Authors Present for Posters Labeled B**

WEDNESDAY, JULY 18, 2012

Morning	Free time to explore the area
12:00 p.m.	*Lunch (included w/registration)*
Probes/Hardware and Methodology - U. Scheler presiding	
1:30 p.m.	**New Trick and Treat in Solid-State NMR.** *K. Takegoshi*, Kyoto University
2:00 p.m.	**Magnetic Resonance Force-Gradient NMR Spectroscopy via Shuttling.** *Doran D. Smith*, US Army Research Laboratory
2:20 p.m.	**Fire Against Fire: Resolution Improvements With the Aid of Couplings?** Lucio Frydman, Weizmann Institute
2:50 p.m.	**Instrumentation and methods development for deuterium NMR of biomolecules.** *Rachel W. M*artin, UC Irvine
3:10 p.m	*Break*
3:30 p.m.	**Multinuclear Solid-State NMR of Organic Molecules: Revealing Intra- and Intermolecular Structure.** *Steven P. Brown*, University of Warwick
4:00 p.m.	**A Common Theory Yields Higher Performance Phase-modulated Homonuclear Dipolar Decoupling.** *Meghan E. Halse*, Université de Lyon (ENS Lyon/CNRS/UNB Lyon1)
4:20 p.m.	**Using NMR to characterise dynamics in molecular solids.** *Paul Hodgkinson*, Durham University
4:50 p.m.	**Recent developments and applications of Magic-Angle Turning.** *Zhehong Gan*, NHMFL
5:10 p.m.	**In Situ High-pressure Variable-temperature NMR for Studies of CO_2 Capture and Sequestration.** *Sophia E. Hayes*, Washington University

THURSDAY, JULY 19, 2012

Dynamic Nuclear Polarization - Z. Gan presiding	
9:00 a.m.	**Structure Property Relations for Catalytic Species on Surfaces by Surface Enhanced NMR Spectroscopy.** *Lyndon Emsley*, Ecole normale supérieure de Lyon
9:30 a.m.	**High-field ^{29}Si, ^{13}C and ^{27}Al Dynamic Nuclear Polarization for the structural characterization of nanoparticles, micro- and meso-porous solids.** *O. Lafon*, Univ. Lille Nord de France
9:50 a.m.	**Many-Spin Coherences in Solid Effect DNP.** *Albert A. Smith*, Massachusetts Institute of Technology
10:10 a.m.	*Break*
10:30 a.m.	**1H Dynamic Nuclear Polarization Based on an Endogenous Radical.** *Anne-Frances Miller*, University of Kentucky
10:50 a.m.	**A Slowly Relaxing Rigid Biradical for Efficient Dynamic Nuclear Polarization Surface-Enhanced NMR Spectroscopy.** *Aaron J. Rossini*, CRMN/ENS Lyon
11:10 a.m.	**Benefits of solid-state dynamic nuclear polarization at below 20 K temperatures.** *Songi Han*, University of California Santa Barbara
11:30 p.m.	**Closing remarks and 2014 Vaughan Lecturer Announcement**