

CEMWOQ-2: Guelph, 10-12 June 2015

2nd Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec

Sponsored by:

Department of Chemistry, CPES and Office of Provost (Academic) at U of Guelph
CrystEngComm • Crystal Growth and Design • Canadian Journal of Chemistry
PANalytical • ATS Scientific • Rigaku Americas
Cambridge Crystallographic Data Centre

Technical Program

CCDC Training Workshop

Wednesday, June 10th
Room SSC-1305

Instructor: Shyam Vyas	
12:30-12:45	Welcome and Introductions
12:45-13:45	Introduction to ConQuest and Mogul Training (Demonstration and Hands on Session)
14:00-14:15	Coffee Break
14:15-15:15	Introduction to Mercury (Demonstration and Hands on Session)
15:15-15:45	Solid Form Module (Presentation and Demo)
15:45-17:00	Twin Track (Solid Form Module - Hands on Session OR Attendees work on their own projects)
17:00	Wrap up

CEMWOQ Day 0 Program

Wednesday, June 10th, 1800

No event is officially scheduled within the CEMWOQ-2 meeting this evening, but we suggest that those who would like to meet other participants walk to the Shakespeare Arms (Pub and Restaurant) after 6 pm with their conference badges on.

CEMWOQ Day 1 Program

Thursday, June 11th

Room SSC-1511

0800	Registration starts
Chair: Kathryn Preuss	
0910 (20 min)	Welcome and Opening Remarks
0930 (30 min)	Travis Holman (Georgetown U) Molecular Materials with Zero-dimensional Pores
1000 (30 min)	Lee Wilson (U of Saskatchewan) NMR Studies of Cyclodextrin/Perfluorinated Guest Compounds
1030	Coffee Break
Chair: Dmitriy Soldatov	
1100 (45 min)	Kenneth Harris (Cardiff U) Towards an Understanding of Molecular Solids: Challenges, Strategies and Solutions
1145 (15 min)	Aaron Smith (U of Guelph) Utilization of the Peptide Matrix: Dipeptides and Beyond (P13)
1200 (15 min)	Michelle Mills (U of Guelph) Supramolecular Host-Guest Structures Employing Lanthanide-Radical Complexes (P12)
1215 (15 min)	Scott Southern (U of Ottawa) Solid-state NMR and Computational Investigations of Non-covalent Tetrel Bonds (P01)
1230	Lunch Break in the Atrium
Chair: Emily Chiang	
1400 (30 min)	David Bryce (U of Ottawa) Applications of NMR Crystallography to Materials
1430 (30 min)	Jeremy Rawson (U of Windsor) Shedding Light on Dithiadiazolyl Radicals: Can You Have Too Much of a Good Thing?
1500 (30 min)	Louis Cuccia (Concordia U) Conglomerate Crystals and Viedma Ripening
1530 (15 min)	David Hirsh (U of Windsor) Characterization of Rare-earth-doped Zeolitic Nanoparticles Using Solid-state NMR (P15)
1545 (15 min)	Katie Psutka (Wilfrid Laurier U) Synthesis and Self-assembly of Discotic Dibenzanthracenedicarboximides and Their Dimers (P03)
1600	Coffee Break
Chair: Kathryn Preuss	
1630 (45 min)	George Shimizu (U of Calgary) MOFs for Clean Energy Applications
1715 (15 min)	Marlon Bridge (Wilfrid Laurier U) A Celebration of Structure: Using the Cambridge Structural Database to Invigorate Undergraduate Concepts (P06)
1730 - 1850	STUDENT POSTER SESSION, Room SSC-1504
1900 - 2200	Reception and Dinner at the Bullring

CEMWOQ Day 2 Program

Friday, June 12th

Room SSC-1511

0800	Registration continues
Chair: Jeremy Rawson	
0900 (30 min)	Graeme Day (U of Southampton) Discovering and Understanding Porous Molecular Crystals by Computational Exploration
0930 (30 min)	Tomislav Friščić (McGill U) Re-discovery of Solid-state Reactivity for Green Synthesis
1000 (15 min)	Jean-Louis Do (McGill U) Solvent-free Mechanochemical Olefin Metathesis: Implications and Applications in the Synthesis of Small Molecules and Macromolecules (P16)
1015 (15 min)	Ivana Brekalo (Georgetown U) Templatation Effects and Novel ZIF Structures by Solid State Synthesis (P08)
1030	Coffee Break
Chair: Tomislav Friščić	
1100 (30 min)	Robert Schurko (U of Windsor)* Multinuclear Solid-State NMR of Pharmaceuticals: Pure, Polymorphic and Dosage Forms
1130 (30 min)	Emily Chiang (U of Guelph) Solid Industrial Waste Material Characterization in View of Valorization
1200 (30 min)	Louise Dawe (Wilfrid Laurier U) A Scaffolded Approach to Learning about Crystallography and Communication in an Undergraduate Chemical Literature Course
1230	Lunch Break in the Atrium
Chair: Robert Schurko	
1400 (30 min)	Holger Eichhorn (U of Windsor) Liquid Crystal and Crystal Engineering of Aromatic Dyes
1430 (30 min)	Kenneth Maly (Wilfrid Laurier U) Engineering Liquid Crystals: Self-Assembly of Novel Polycyclic Aromatic Hydrocarbons
1500 (30 min)	Closing Remarks and Student Awards
1530	Coffee Break
1600	Extended Executive Meeting, Room SSC-1508

* All authors: RW Schurko, MJ Jaroszewicz, AM Namespetra, A Sandre, MP Hildebrand, H Hamaed, SL Veinberg, KE Johnston, L Frydman, M Pruski, T Kobayashi, I Hung and Z Gan

Color Key:

(45 min)	Plenary Lecture
(30 min)	Invited Lecture
(15 min)	Student Flash Talk

Student Poster Session
Thursday, June 11th, 1730 - 1850
Room SSC-1504

P01

Scott Southern, David Bryce (U of Ottawa)

"Solid-state NMR and Computational Investigations of Non-covalent Tetrel Bonds"

P02

Andy Tsang, Farukh I Ali, Dmitriy V Soldatov (U of Guelph)

"2,5-Diketopiperazines for the Design of Pharmaceutically Relevant Co-crystals"

P03

Katie M Psutka, Kenneth E Maly (Wilfrid Laurier U)

"Synthesis and Self-assembly of Discotic Dibenzanthracenedicarboximides and Their Dimers"

P04

Michael Reynolds, Kenneth E Maly (Wilfrid Laurier U)

"Self-assembly of Dibenzopentacenequinones in Columnar Mesophases and the Solid State"

P05

Jeffrey Dinsmore, Louise Dawe (Wilfrid Laurier U)

"Prevention instead of Retraction: Integrating Learning Outcomes Related to Ethical Practices in Undergraduate Studies"

P06

Marlon Bridge, Negeen Foroughian, Louise Dawe (Wilfrid Laurier U)

"A Celebration of Structure: Using the Cambridge Structural Database to Invigorate Undergraduate Concepts"

P07

Aldo Van Audenaerde, Yi Wai Chiang, Rafael Santos, Remus Ion Iacobescu, Tom Van Gerven, Emily Chiang (U of Guelph)

"Finding Nickel in Olivine"

P08

Ivana Brekalo, Christopher M Kane, Joseph R Ramirez, K Travis Holman (Georgetown U)

"Templation Effects and Novel ZIF Structures by Solid State Synthesis"

P09

Travis AP Fillion, Dmitriy V Soldatov, Kathryn E Preuss (U of Guelph)

"Lanthanide-based Coordination Polymers and Their Use in the Rational Design of Porous Metal-organic Frameworks"

P10

Farukh I Ali, Dmitriy V Soldatov (U of Guelph)

"H-Bonded Tapes of 2,5-Diketopiperazines: Novel Candidate for the Design of Co-crystals"

P11

R Alex Mayo, David J Sullivan, Travis AP Fillion, Dmitriy V Soldatov, Kathryn E Preuss (U of Guelph)

"Conformational Polymorphism of a 1,2,3-DTA Ligand"

P12

Michelle B Mills, Andrew Hollingshead, Adam C Maahs, Dmitriy V Soldatov, Kathryn E Preuss (U of Guelph)

"Supramolecular Host-Guest Structures Employing Lanthanide-Radical Complexes"

P13

Aaron J Smith, Melissa Ignacio, Travis AP Fillion, Dmitriy V Soldatov (U of Guelph)

"Utilization of the Peptide Matrix: Dipeptides and Beyond"

P14

Michael J Jaroszewicz, Anthony R Sandre, Andrew M Namespetra, Stanislav L Veinberg, Karen E Johnston, Zhehong Gan, Ivan Hung, Robert W Schurko (U of Windsor)

"Spectral Editing in Ultra-wideline NMR: Detection of Polymorphs and Impurity Phases in Solid Pharmaceuticals"

P15

David A Hirsh, Bryan EG Lucier, Anna M Ritcey, Robert W Schurko (U of Windsor)

"Characterization of Rare-earth-doped Zeolitic Nanoparticles Using Solid-state NMR"

P16

Jean-Louis Do, Tomislav Friscic (McGill U)

"Solvent-free Mechanochemical Olefin Metathesis: Implications and Applications in the Synthesis of Small Molecules and Macromolecules"

P17

Rui Sun, Igor Huskic, Tomislav Friscic (McGill U)

"Low-energy and Solvent-free Activation of Metal Oxides and Solid-state Separation of Lanthanide Oxides"

P18

Adam C Maahs, Dmitriy V Soldatov, Kathryn E Preuss (U of Guelph)

"Plastic Bending Crystals of 2-Cyano-4,6-dimethylpyrimidine"

P19

Ellen Song, Michelle B Mills, Dmitriy V Soldatov, Kathryn E Preuss (U of Guelph)

"Synthesis of Iron(II) Spin Crossover Complexes with Thiazyl Radicals"

P20

Alexander J Stirk, Kelong Zhu, Stephen J Loeb (U of Windsor)

"Utilising Void Space: T-Shaped Rotaxane Ligands for MOFs"

P21

Christopher W Nickels, Cristina Mottillo, Simon Girard, Tomislav Friscic, Chao-Jun Li (McGill U)

"New Methods in Post Synthetic Processing of Metal-organic Frameworks"

P22

Lee D Wilson, Mohamed H Mohamed, John V Headley (U of Saskatchewan)

"Tuning the Physicochemical Properties of Polysaccharides via Cross-linking Conditions"