The 6th Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec

May 30th – June 1st, 2019
Montréal, Quebec

Université
Concordia
University

Conference Venue

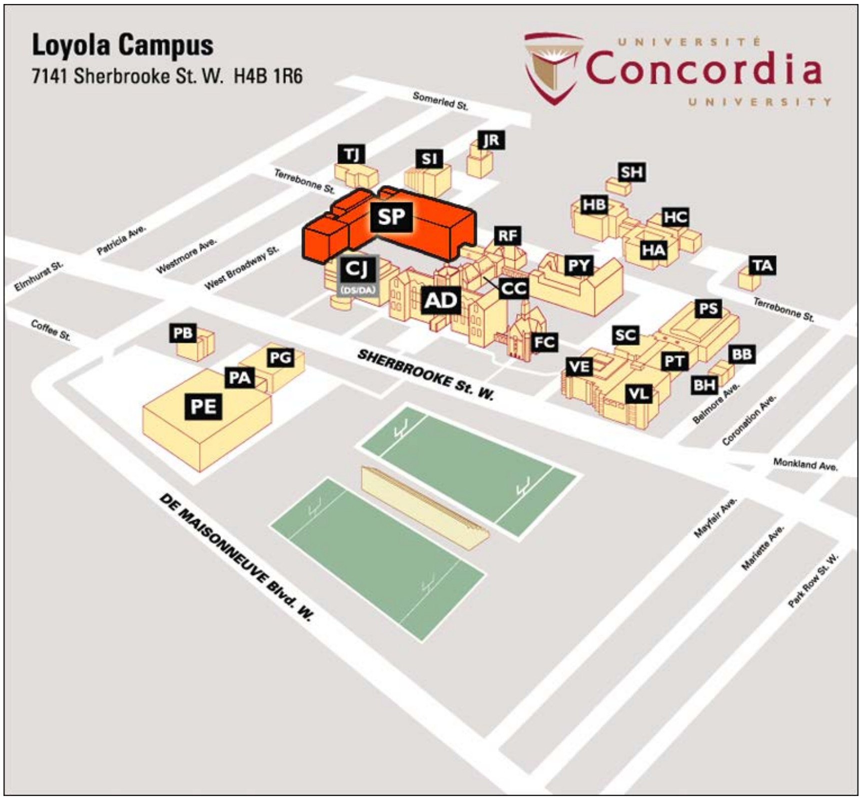
CEMWOQ-6 will take place on the Loyola Campus of Concordia University – in the Loyola Jesuit Hall and Conference Centre (Labelled “RF” on the map below, next to the Science Pavilion "SP").

Please note that the workshops, and all invited and contributed talks will be held in room SP S110, whereas the food, sponsors exhibit, and poster presentation sessions are located in the RF Center.

If you are staying in downtown Montreal, you can ride the Concordia shuttle bus from our downtown campus to the conference venue for free. Just mention to the driver that you are attending the CEMWOQ-6 workshop.

On Thursday and Friday, the shuttle bus will depart from 1455 De Maisonneuve Blvd. W. (The front doors of the Hall Building). The shuttle will depart at 8:55am, 9:30am and every 35 minutes after. You can also ride the shuttle bus home at 8:05pm or 8:35pm (this is the last departure from Loyola Campus to downtown).

On Saturday, there will be one shuttle bus which will depart from the Grey Nuns Residence at 9:00am. All attendees must find their own transportation back to downtown on Saturday.



Organizing Committee

Ashlee J. Howarth

Ashlee J. Howarth is an Assistant Professor of Chemistry at Concordia University in Montréal. Professor Howarth graduated from the University of Western Ontario in 2009 with an Honours BSc in Chemistry and then went on to do her PhD in inorganic materials chemistry at the University of British Columbia. Before joining the faculty at Concordia, she completed an NSERC Postdoctoral Fellowship at Northwestern University, where she worked primarily on the design and synthesis of MOFs for applications in wastewater remediation. She was recently recognized by Forbes Magazine as a "30 under 30" in Science. Research in the Howarth group at Concordia University focuses on designing new MOFs for green applications.

Louis Cuccia

Prof. Louis Cuccia earned his PhD (1997) at McGill University studying the biophysical properties of bipolar phospholipids under the supervision of Prof. Bruce Lennox. Prior to joining Concordia University (2002), he carried out postdoctoral research in supramolecular chemistry at Université Louis Pasteur (Strasbourg, France) and studied advanced scanning probe microscopy techniques at the Steacie Institute for Molecular Sciences (NRC) in Ottawa. He is currently an Associate Professor at Concordia with an enthusiastic group of graduate and undergraduate students carrying out research on topics ranging from chiral crystals and chiral amplification to supramolecular chemistry and surface self-assembly.

Paola Marino

Paola Marino is a fourth year undergraduate student completing her B.Sc. Specialization in Biochemistry at Concordia University in Montréal. She joined the Howarth Research Group in February 2018 due to her interest in the synthesis, functionalization and applications of metal–organic frameworks (MOFs). Her research interests are related to environmental and health sciences and devoted to green chemistry and pharmacology. Her involvement in the MOF community increased by participating in the 5th annual Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec (CEMWOQ-5), and for this years workshop, CEMWOQ-6, she joined the organizing committee to have a more involved role in this valuable educational and networking event.

Zvart Ajoyan

Zvart Ajoyan is an undergraduate student in the department of Chemistry & Biochemistry at Concordia University. She is in her fourth year completing her B.Sc. Specialization in Biochemistry. Her research interests include MOF chemistry pertaining to green chemistry. She joined the Howarth Research Group in February 2018, to further pursue her interests and to develop her knowledge in the field of metal–organic frameworks. She joined the organizing committee of the 6th annual crystal engineering and emerging materials workshop of Quebec and Ontario (CEMWOQ-6) to be more involved in the crystal engineering and MOF community in Canada.

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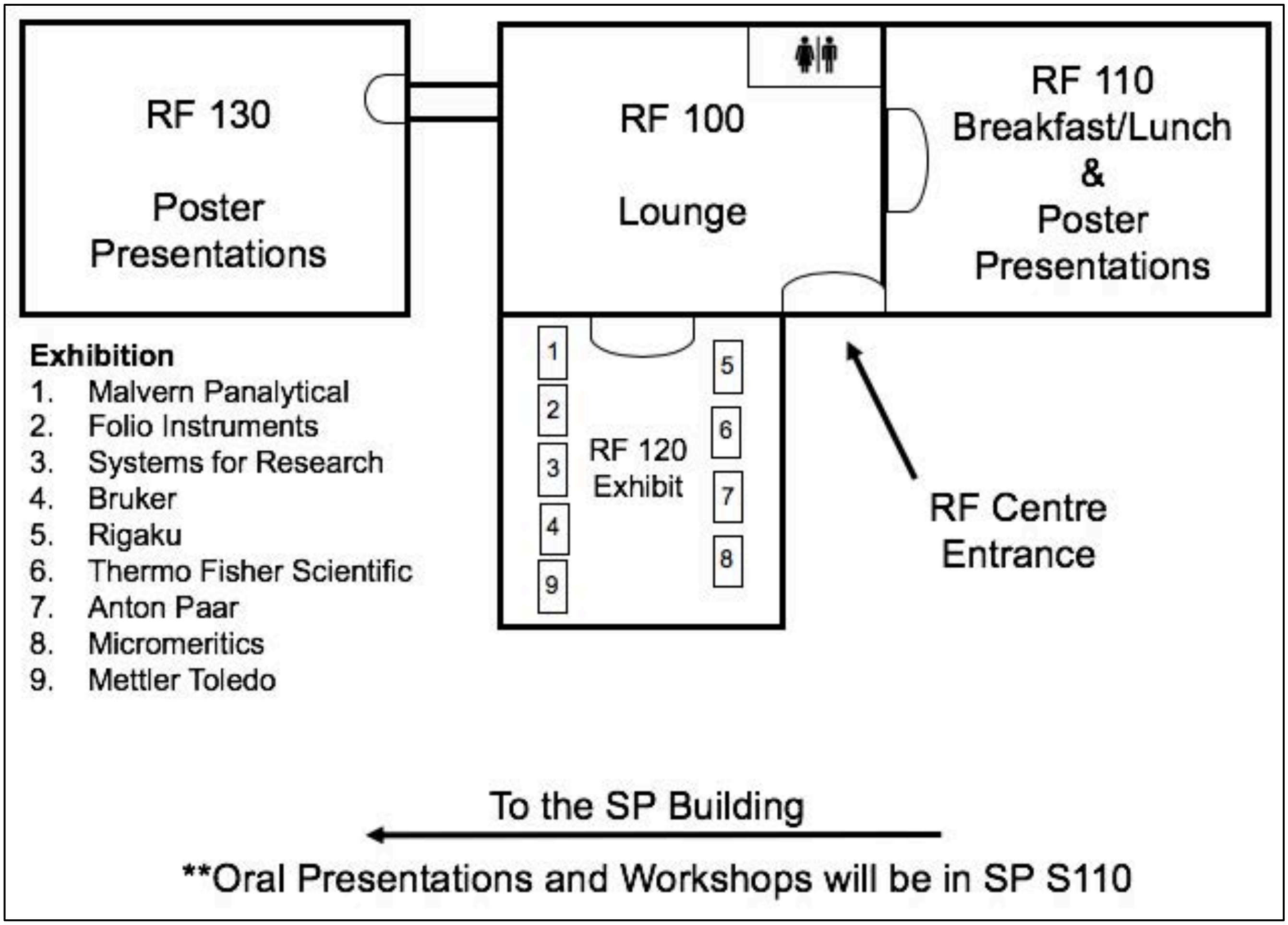
CEMWOQ-6 is grateful for the financial support received from the Department of Chemistry and Biochemistry, the Faculty of Arts and Science and the Office of the Vice-President, Research & Graduate Studies.

Thank you to our sponsors!

Exhibition Layout



Exhibition
1. Malvern Panalytical
2. Folio Instruments
3. Systems for Research
4. Bruker
5. Rigaku
6. Thermo Fisher Scientific
7. Anton Paar
8. Micromeritics
9. Mettler Toledo

**Oral Presentations and Workshops will be in SP S110

Breakfast, Lunch, and Conference Dinner

Breakfast will be provided to participants during the scheduled times in the morning on Thursday, Friday, and Saturday (May 30th – June 1st).

Lunch meals will be provided to participants during the scheduled lunch breaks on Thursday, Friday, and Saturday (May 30th – June 1st).

The CEMWOQ-6 Conference Dinner will be held at Hotel Le Crystal on Friday, May 31st after the poster presentation sessions, and the bus provided for transportation to the dinner venue will depart from the Loyola Campus at 7:00pm.

Conference Dinner Venue Address:

Hotel Le Crystal
1100 Rue de la Montagne
Montréal, QC
H3G 0A1

Meeting Program

Thursday, May 30th			
10:00 am	-	10:45 am	Registration and Breakfast from Pekarna Catering
10:45 am	-	11:45 am	**Workshop #1** **Michael Katz** (Memorial University of Newfoundland) *"Gas Adsorption and Isotherm Fitting"*
11:45 am	-	1:00 pm	Lunch Break
1:00 pm	-	2:00 pm	**Workshop #1 (cont'd)** **Michael Katz** (Memorial University of Newfoundland) *"Gas Adsorption and Isotherm Fitting"*
2:00 pm	-	2:15 pm	Coffee Break
2:15 pm	-	4:00 pm	**Workshop #2** **Amy Sarjeant** (Cambridge Crystallographic Data Centre) *"Data Mining with ConQuest and Mercury"*
4:00 pm	-	4:15 pm	Short Break
4:15 pm	-	4:30 pm	Welcome Comments
Chair, Joseph Ricardo-Noordberg, Graduate Student, Concordia University			
4:30 pm	-	5:00 pm	**Invited Talk**: **Marc McKee** (McGill University) *"Life at a crystal's edge: The organic-inorganic interface in biomineralization"*
5:00 pm	-	5:20 pm	**Jennifer Murphy** (Memorial University of Newfoundland) *"How calcite 'musseled' its way into supercapacitors"*
Chair, Chris Copeman, Undergraduate Student, Concordia University			
5:20 pm	-	5:40 pm	**Igor Huskić** (McGill University) *"Proton Conductivity and Polymorphism in Organic Minerals and Their Analogues"*
5:40 pm	-	6:10 pm	**Invited Talk**: **Georges Dénès** (Concordia University) *"When crystals grow only in low dimensions"*
6:10 pm	-	7:00 pm	Poster Session **A**
7:00 pm	-	7:50 pm	Poster Session **B**

Friday, May 31st			
9:30 am	-	10:00 am	Registration and Breakfast from Pekarna Catering
Chair, Zvart Ajoyan, Undergraduate Student, Concordia University			
10:00 am	-	10:30 am	**Invited Talk**: **Nicholas Vukotic** (PROTO Manufacturing & University of Windsor) *“From Academia to Industry to Synergy”*
10:30 am	-	10:50 am	**Novendra Novendra** (University of California, Davis) *“Experimental Evaluation of Substitution Effect on Thermodynamic Stability of Zeolitic Imidazolate Frameworks”*
10:50 am	-	11:10 am	**Hatem Titi** (McGill University) *“Greener hypergolic solid fuels for aerospace application”*
Chair, Carmen Yan, Undergraduate Student, Concordia University			
11:10 am	-	11:40 am	**Invited Talk**: **Michael Katz** (Memorial University of Newfoundland) *“Feeling our way through crystal engineering toward applications of framework materials”*
11:40 am	-	12:00 pm	**Shefa Alomari** (Clarkson University) *“Design and Synthesis of Zwitterionic Metal–Organic Frameworks”*
12:00 pm	-	1:30 pm	Lunch Break
Chair, Felix Saraci, Graduate Student, Concordia University			
1:30 pm	-	2:00 pm	**Invited Talk**: **Ronald Rubinovitz** (Thermo Fisher Scientific) *“The Use of FTIR in the Characterization of Crystal Structures”*
2:00 pm	-	2:20 pm	**Juby Varghese** (Clarkson University) *“Metal–Organic Frameworks as Platforms for the Nanostructuration of Single Molecule Magnets: New Insights from HRTEM”*
Chair, Victor Quezada, Graduate Student, Concordia University			
2:20 pm	-	2:40 pm	**Zineb Ras Ali** (Brock University) *“Synthesis and magneto-structural studies of 4f complexes of dibenzo15C5 macrocycles”*
2:40 pm	-	3:10 pm	**Invited Talk**: **Muralee Murugesu** (University of Ottawa) *“Dynamic guest adsorption visualized through crystal free crystallography”*
3:10 pm	-	3:30 pm	**Dominique Leckie** (University of Windsor) *“Transition Metal Complexes of the 1,3,2-Dithiazolyl Radical”*
3:30 pm	-	4:00 pm	Coffee Break

Chair, Zujhar Singh, Graduate Student, Concordia University			
4:00 pm	-	4:30 pm	**Invited Talk**: **Michael O. Wolf** (University of British Columbia) *“Photofunctional sulfur-bridged conjugated materials”*
4:30 pm	-	4:50pm	**Lara Watanabe** (University of Windsor) *“Investigation between the mononuclear and dinuclear transformation of cobalt dithiolates”*
Chair, Adriana Danko, Undergraduate Student, Concordia University			
4:50 pm	-	5:10 pm	**Lana Hiscock** (Wilfrid Laurier University) *“Synthesis, Characterisation, and Photophysical Properties of a Series of 6,13-Dicyanoheteropentacene Analogues”*
5:10 pm	-	5:40 pm	**Invited Talk**: **Sally Brooker** (University of Otago) *“Spin Crossover”*
5:40 pm	-	6:20 pm	Poster Session **B**
6:20 pm	-	7:00 pm	Poster Session **A**
7:00 pm			Bus Leaves for Conference Dinner

Saturday, June 1st

9:30 am	-	10:00 am	Breakfast from Pekarna Catering
Chair, Zvart Ajoyan, Undergraduate Student, Concordia University			
10:00 am	-	10:30 am	**Invited Talk**: **Ngong Kodiah Beyeh** (Oakland University) *“Self-Assembly of Biohybrid Materials with Macrocyclic Receptors”*
10:30 am	-	10:50 am	**Alex Mayo** (Solid State Pharma Inc.) *“Improving Experimental Success of Co-Crystallization with Computational Pre-Screening of Co-Formers”*
Chair, Malik Ammad Iqbal, Undergraduate Student, Concordia University			
10:50 am	-	11:10 am	**Austin Peach** (University of Windsor) *“What Can Multi-Component Milling Tell Us About Fluoxetine HCl Cocrystals?”*
11:10 am	-	11:40 am	**Invited Talk**: **Joseph D. Ferrara** (Rigaku Americas Corporation) *“Thirty-Five Years of Crystallography: An Industrial Perspective”*
11:40 am	-	12:00 pm	**Colum O’Connor** (Cranfield University) *“Co-crystals: Designer explosives for the future”*
12:00 pm	-	1:30 pm	Lunch Break

Chair, Joseph Ricardo-Noordberg, Graduate Student, Concordia University	
1:30 pm - 2:00 pm	**Invited Talk**: **Eva Hemmer** (University of Ottawa) *“From Nano to Micro – Synthesis and Optical Characterization of Rare-Earth-based Materials”*
2:00 pm - 2:20 pm	**Sina Mirzaeifard** (McGill University) *“Simulation and Modeling of the Interface between the Liquid Water and Methane Hydrate Crystal”*
2:20 pm - 2:40 pm	**Sean Holmes** (University of Windsor) *“NMR crystallography of active pharmaceutical ingredients and nutraceuticals: Insights into crystal structure from dispersion-corrected DFT calculations”*
Chair, Reginald Gratia, Undergraduate Student, Concordia University	
2:40 pm - 3:10 pm	**Invited Talk**: **Anna Gudmundsdottir** (University of Cincinnati) *“Towards Understanding the Photodynamic Behavior of Vinyl Azides Crystals”*
3:10 pm - 3:30 pm	**Ivana Brekalo** (Georgetown University) *“Are guanidinium sulfonates formally microporous”*
3:30 pm - 4:00 pm	Coffee Break
Chair, Paola Marino, Undergraduate Student, Concordia University	
4:00 pm - 4:30 pm	**Invited Talk**: **Fiorenzo Vetrone** (INRS-EMT, Université du Québec) *“Controlling the Nanoscale Architecture in Rare Earth Doped Nanocrystals”*
4:30 pm - 5:30 pm	**Plenary Lecture**: **Andy Cooper** (University of Liverpool) *“Discovering functional materials by fusing de novo prediction with autonomous robotics”*
5:30 pm - 6:00 pm	Wrap up and Awards: Ashlee, Louis, Paola, and Zvart

Posters in RF 110
Poster Session A = Even-Numbered Posters
Poster Session B = Odd-Numbered Posters

Poster Number	Name	Affiliation	Title
1	Blaine Fiss	McGill University	Mechanochemical Phosphorylation of Polymers and Synthesis of Flame-Retardant Cellulose Nanocrystals
2	Cameron Lennox	McGill University	Ultralight main-group imidazolate frameworks
3	Cameron Vojvodin	University of Windsor	NMR Crystallography of Multi-Component Crystals Containing Urea
4	Carmen Yan	Concordia University	Zirconium and Yttrium mixed-metal–organic frameworks
5	Chris Copeman	Concordia University	Carbonate Loaded MOF-808 for Wastewater Remediation
6	Daniel Therien	McGill University	Mechanoenzymatic breakdown of chitin into N-acetylglucosamine in the absence of bulk solvent
7	Filip Topić	McGill University	Efficient recognition of steroids by planar aromatic molecules: Exploring the building block landscape and potential applications of a novel biomolecular recognition motif
8	Hudson Bicalho	Concordia University	Development of Eu- and Zr-MOFs for Environmental Applications
9	Joseph Ricardo-Noordberg	Concordia University	An Inexpensive Photochemical Cell Towards the Photocatalytic Generation of High Value-Added Chemicals
10	Kayrel Edwards	McGill University	Preparing cellulose-based stimuli responsive hydrogen-bonded materials
11	Love Karan	Université du Québec à Trois-Rivières	Efficient amide based luminescent metal–organic hybrids for selective detection of mycotoxins in food samples: Synthesis of hybrids and detection of toxins using photoluminescence studies
12	Maria Matlinska	University of Alberta	Exploring Hydrogen Boding in Solids: Atomic Level Insight with Solid-State NMR
13	Mihails Arhangelskis	McGill University	Ab initio structure prediction of metal–organic frameworks
14	Mitchell Nascimento	University of Victoria	Ring-Opening Polymerization of Cyclic Phosphonates: Access to Inorganic Polymers with a P(V)–O Main Chain
15	Mohini Ramkaran	McGill University	McGill Chemistry Characterization (MC^2) Facility
16	Nadia Stephaniuk	University of Windsor	Crystal Engineering of Thiazyl-based Radical-Radical Co-Crystals
17	Nour Dissem	Institut de Recherche sur l'Hydrogène UQTR	Synthesis and characterization of a new Cu(II) 3D coordination polymer from a mixed ligand synthetic approach
18	Olivier Schott	Université de Montréal	Supramolecular photochemistry towards solar hydrogen generation: Ir and Ru photosensitizers with Cobaltoximes
19	Patrick Julien	McGill University	Monitoring Mechanochemical synthesis of cocrystal fertilizers reveals water mediated feedback mechanism
20	Szymon Sobczak	Adam Mickiewicz University	Mass spectrometry as a tool for controlling products of high-pressure disulphide metathesis reaction
21	Tomislav Friščić	McGill University	Remembering Joel Bernstein: The archetype of cocrystal-mediated solvent-free synthesis
22	Victor Quezada	Concordia University	A New Metal–Organic Framework synthesized from Yttrium and a Tetratopic Linker
23	Zachary Schroeder	Wilfrid Laurier University	Synthesis of Polycyclic Aromatic Hydrocarbons via Yamamoto Cyclization

Posters in RF 130
Poster Session A = Even-Numbered Posters
Poster Session B = Odd-Numbered Posters

Poster Number	Name	Affiliation	Title
24	Abdullah Abudayyeh	University of Otago	Visible Light–Driven Reduction Of H^+ or CO_2 Catalysed By Cobalt Macrocycles
25	Adriana Danko	Concordia University	Stability of Zr-UiO-66 Metal–Organic Frameworks in Aqueous Environments under Varying pH Conditions
26	Alicia McTaggart	Concordia University	The role of pH in the growth of silica-carbonate microstructures
27	Felix Saraci	Concordia University	Rare-earth Metal–Organic Frameworks (RE-MOFs) as fluorescent-based chemical sensors for applications in the detection of antibiotic contaminants in water
28	Francisco Yarur	Concordia University	Visible-Light Sensitization of Inorganic Semiconducting Nanostructures for Photoelectrochemical Energy Conversion
29	Ghada Ayoub	McGill University	Mechanochemistry, accelerated aging, or both? Solid-state synthesis of edible MOFs
30	Jean-Louis Do	Concordia University / McGill University	Exploiting the Flexible Interactions of Salicylic Acid-Based Helicates in the Synthesis of New Metal–Organic Materials
31	Jogirdas Vainauskas	McGill University	Engineering Azulene-based Dichroic Cocrystals Using Halogen Bonding
32	John Hadynski	Clarkson University	Design and Synthesis of Zwitterionic Metal–Organic Frameworks
33	Joseph Marrett	McGill University	Modulation of hypergolic behavior in MOFs via changes in solid-state structure
34	Louae Abdulla	University of Windsor	Polymorphism in Xylazine HCl: A Solid-State NMR and DFT Study
35	Mehdi Esmaeili	University of Guelph	Short peptides as building blocks for soft materials
36	Midhun Mohan	Université du Québec à Trois-Rivières	Synthesis of Novel Pyridone-based Metal–Organic Framework
37	Mohammad Sharif Askari	Concordia University	Sodium Chlorate and Mirror Symmetry Breaking – A Historic Perspective
38	Monu Joy	Clarkson University	Metal–Organic Frameworks as Platforms for the Nanostructuration of Single Molecule Magnets: New Insights from HRTEM
39	Paola Marino and Zvart Ajoyan	Concordia University	Functional Hexanuclear Cluster-Based Metal–Organic Frameworks: From Materials Design to Application
40	Pedro Donnarumma	Concordia University	Rare-earth based **fcu** Metal–Organic Frameworks for aqueous contaminants degradation
41	Petr Fiurasek	Québec Centre for Advanced Materials	Centre Québécois sur les Matériaux Fonctionnels (CQMF) - Quebec Centre for Advanced Materials (QCAM)
42	Oliver Bleton, Ismael Elhasadi, and Amandeep Thind	Concordia University	Materials and Pharmaceutical Applications of Chiral Supramolecular Assemblies
43	Robin Stein	McGill University	McGill Chemistry Characterization (MC^2) Facility
44	Sandra Kaabel	McGill University	Anion-templated dynamic covalent self-assembly of hemicucurbit[n]uril macrocycles in the solid state
45	Sanil Rajak	Université du Québec à Trois-Rivières	Catalyst Design For Photochemical Hydrogen Evolution Reaction
46	Zahir Razzaz	Laval University	Production and characterization of hollow fiber extruded foam membranes for gas separation
47	Zujhar Singh	Concordia University	Synthesis and integration of donor-chromophore-acceptor (D-C-A) based Cu(I) triads onto semiconductor surfaces to drive single electron transfer (SET) processes

Workshops

The workshops are held in room SP S110

Thursday Workshop:
Dr. Amy Sarjeant, General Manager
Cambridge Crystallographic Data Centre

The CCDC is pleased to present a 2-hour workshop on the Cambridge Structural Database and our software tools. We'll focus on structure searching and data mining with ConQuest and Mercury, and delve into various ways to investigate intra- and intermolecular interactions in the solid state.

Thursday Workshop:
Prof. Michael J. Katz, Assistant Professor
Memorial University of Newfoundland

Gas adsorption is one of the primary ways to measure the porosity of a material. Currently, instrumentation is capable of collecting data and returning information on the surface area, pore sizes, and isosteric heats of adsorption. This workshop will focus on taking a step back from the automated process in order to discuss the principles behind the instrumentation as well as the theories used to convert isotherm data into surface area, pore sizes, and isosteric heats of adsorption.

All CEMWOQ-6 attendees are welcome to attend the workshops

Abstracts of Invited Talks

The invited talks are held in room SP S110

Plenary Lecture

Prof. Andy Cooper
University of Liverpool

Discovering functional materials by fusing de novo prediction with autonomous robotics

Porous molecular crystals are an alternative to porous extended frameworks such as zeolites, metal–organic frameworks (MOFs), covalent organic frameworks (COFs), and polymer networks. Interest in such systems predates MOFs, tracing back to Barrer's first 'organic zeolites', but only recently have molecular crystals started to show physical properties that are competitive with extended, bonded frameworks.

However, molecular crystals—porous or otherwise—pose problems in terms of the purposeful design of function. This is because the energy landscape for molecular crystals is typically not dominated by a single intermolecular interaction, unlike bonded crystalline frameworks. Hence, molecular crystal engineering has so far failed to become the "new organic synthesis" that was envisaged, and extended, bonded frameworks have recently dominated the scene. They do not follow the isoreticular scheme that defines the strategy for MOFs and COFs.

This lecture will discuss the design and synthesis of new functional organic crystals using computationally-led approaches. In particular, we will discuss a new approach for designing function in molecular crystals, based on knowledge of the building blocks alone, by constructing "energy–structure–function maps". I will show that this design strategy works for both known molecules and for hypothetical molecules that have not yet been made in the laboratory. I will also outline our future vision for the direct integration of materials properties predictions with mobile laboratory robots, thus allowing the semi-autonomous discovery of new materials with properties that would be hard to access by more conventional methods.

Prof. Anna D. Gudmundsdottir
University of Cincinnati

Towards Understanding the Photodynamic Behavior of Vinyl Azides Crystals

The quest for sustainable chemistry is reinforcing interest in solid-state photochemistry as a sustainable tool for synthetical applications because organic crystals can be used to carry out photoreactions without solvents and most photoreactions can be initiated by sunlight or photocatalysts.[1] In particular, solid-state photoreactions are generally more regio- and stereoselective than their solution counterparts, because the rigid packing of molecules in the crystal lattice prevents significant rotation and diffusion.[2] In contrast, recent findings highlight that organic crystals can also be flexible and compression can make them bend, curl, hop, or twist when exposed to light or external pressure.[3] Thus, photodynamic crystals can convert light into mechanical energy, and they have a potential role in the fabrication of mechanically tunable components for actuation, energy harvesting, flexible electronics, and switchable reflectors. In addition, such crystals can be used as sensors and probes.

We have shown that photolysis of azido derivatives results in formation of triplet nitrenes and N_2 gas. The release of N_2 molecules from the crystal lattice is distinctive for each azido derivative. For example, some crystals tolerate a build-up of large N_2 bubbles within the crystals before cracking, whereas others shatter fiercely upon exposure to light. The behavior of azido crystals and their solid-state reaction mechanisms will be discussed and correlated to the azido crystal packing arrangements.

[1] (a) Skubi, K. L.; Blum, T. R.; Yoon, T. P., Chem. Rev. 2016, 116, 10035-10074; (b) Staveness, D.; Bosque, I.; Stephenson, C. R. J., Acc. of Chem. Res. 2016, 49 (10), 2295-2306; (c) Schultz, D. M.; Yoon, T. P. Science 2014, 343 (6174).
[2] Ramamurthy, V.; Venkatesan, K. Chem. Rev. 1987, 87 (2), 433-481.
[3] Naumov, P.; Chizhik, S.; Panda, M. K.; Nath, N. K.; Boldyreva, E. Chem. Rev. 2015, 115 (22), 12440-12490.

Prof. Eva Hemmer
University of Ottawa

From Nano to Micro – Synthesis and Optical Characterization of Rare-Earth-based Materials

Based on their outstanding optical properties, Ln^{3+}-based compounds have been suggested for a wide range of applications including the fields of biomedicine, optoelectronics, and solar energy conversion. For instance, the capability of Ln^{3+}-based materials to emit visible and near-infrared (NIR) light under NIR excitation is highly sought after when aiming for biomedical applications. This is due to the fact that NIR light penetrates deeper into biological tissue when compared to UV or visible light. Fluorides of the general composition $MREF_4$ (M = alkali metal, RE = rare earth), are commonly considered as suitable host materials for upconverting and NIR emitting Ln^{3+} ions (e.g. Er^{3+}, Tm^{3+}, Ho^{3+}). The microwave-assisted approach offers a promising alternative for the synthesis of $MREF_4$ particles spanning the nano to micro scale. This presentation will shine a light on the versatile landscape of RE^{3+}-based materials focusing on materials synthesis and RE^{3+}-specific optical features.

Prof. Fiorenzo Vetrone
INRS-EMT, Université du Québec

Controlling the Nanoscale Architecture in Rare Earth Doped Nanocrystals

Rare earth doped nanocrystals (RENCs) possess fascinating optical properties due to the multitude of long lived 4f electronic energy states. As a result, they can be excited as well as emit light at wavelengths spanning the UV to the near-infrared. Over the last few years, advancements in our understanding of the synthetic techniques has allowed for the development of RENCs with architectures that permit for precise and selective doping of the rare earth ions in different components of the nanocrystal architecture. Such controlled doping has resulted in the unprecedented ability to manipulate the optical properties of the RENCPs potentially charting a course leading to new applications in diverse fields such as energy, environment and health. Here, we will give an overview of RENCs as well as present a perspective on the role of the nanoarchitecture on their optical properties and subsequently in different biomedical applications.

Prof. Georges Dénès
Concordia University

When crystals grow only in low dimensions

Authors:
Georges Dénès, M. Cecilia Madamba, Juanita M. Parris, Abdualhafed Muntasar and Hocine Merazig

Crystal growth can be very frustrating. While some species grow easily in nice three-dimensional crystals, others stubbornly refuse to grow at all beyond the tiny size of powdery particles. There are also some species that grow in one- or two-dimensions to give needles or plalelet-shaped crystals. We have investigated over several decades a large number of divalent tin compounds, with various degrees of success in growing crystals. Most of the crystals obtained are one- or two-dimensional. The presentation will show that the stereoactivity of the tin(II) lone pair, and its orientation in space when it is stereoactive, determines the dimensionality of the crystal growth. In addition, the absence of large enough crystals for single crystal diffraction, or their insufficient quality due to their low-dimensionality, has prompted us to find other methods to help solving crystal structures. The presentation will show that the combination of X-ray powder diffraction and tin-119 Mössbauer spectroscopy was very successful in many cases.

Dr. Joseph D. Ferrara
Rigaku Americas Corporation

Thirty-Five Years of Crystallography: An Industrial Perspective

In 1984, we were using diffractometers with point detectors for data collection, mainframe computers for data analysis, flat bed plotters for graphics and overhead projectors for presentations, thus, a data set might take a few days and run as long a month, a cycle of least squares refinement might take an hour to a week, a plot might take all afternoon and the latest results would be handwritten on a sheet of plastic. Today we are using systems that are a thousand times more powerful, distributed over many more sites, allowing us to handle complicated problems easily. In this presentation, I will review how crystallography has evolved since 1984 and look toward the future.

Prof. Marc D. McKee
McGill University

Life at a crystal's edge: The organic-inorganic interface in biomineralization

Reconciliation of the evolving interplay between organic moieties and inorganic crystals lies at the heart of modern biomineralization inquiry. Recent biomineralization research in vertebrates has identified, characterized and described functions for key noncollagenous extracellular matrix proteins regulating crystal growth in the skeleton and dentition by binding to mineral. Gene mutations affecting mineral-regulating proteins typically lead to bone and tooth nanocrystallites defective in number, size, shape and/or orientation, and can even potentially lead to changes in mineral type, such that these otherwise hard tissues become diseased, soft and/or brittle. Several bone and tooth diseases will be discussed in terms of altered molecular determinants of mineralization. Some of these same proteins expressed in soft tissues undergoing pathologic calcification (like blood vessels) also inhibit ectopic crystal growth. In calcium carbonate biomineralizing systems like inner ear otoconia and avian eggshells, similar proteins likewise regulate mineralization. In addition to peptides and proteins, we also show that calcium carbonate (vaterite) chirality effects can be induced by chiral acidic amino acids in an in vitro crystal growth system, leading to formation of synthetic, hierarchically organized, helicoidal extended suprastructures. Rational use of these enantiomeric effects will allow for the design of novel mineral crystal-containing, composite/hybrid chiroptical and biologically active materials.

This work was funded by CIHR and NSERC.

Prof. Michael J. Katz
Memorial University of Newfoundland

Feeling our way through crystal engineering toward applications of framework materials

Crystal engineering is rarely a linear process from design to application. This is especially true in the synthesis of Metal–Organic Frameworks (MOFs) where reagents, modulators, and solvents are sealed in a vessel, tossed (albeit gently) into an oven and examined every few hours, days, or weeks. The challenge is that seemingly insignificant changes and differences can have profound fluctuations on MOF formation. With considerable work focusing on the application of MOFs, the details of the successes and failures associated with the synthesis are often not explored. This can often lead young researchers to believing that they don’t have synthetic hands when, in reality, an unknown variable that authors didn’t explore and/or readers didn’t consider important are at play. This talk will illustrate some of our struggles, successes, failures, and fortunate missteps on our way from design to applications of MOFs.

Prof. Michael O. Wolf
University of British Columbia

Photofunctional sulfur-bridged conjugated materials

Authors:
Jennifer Yuan, Peter Christensen and Michael O. Wolf

Sulfur-based bridging groups (sulfides, sulfoxides and sulfones) provide a convenient, tunable approach to varying the electronic behaviour of pi-functional materials. The photophysical and photochemical behavior of several classes of sulfur-bridged materials will be described. Symmetric chromophore dimers are of interest for applications in optoelectronic devices as they offer the potential for optimization of energy and charge transfer processes. A series of sulfur-bridged chromophore dimers in which the intradimer electronic coupling can be varied by changing the oxidation state of the bridging sulfur group will be discussed. We show that excited state charge transfer character can be varied by tuning the bridge oxidation state. Steady-state and time-resolved spectroscopy, in combination with computational results are used to evaluate the electronic structure of these dimers. Applications of these systems in optoelectronic devices will be discussed, and polymers containing these functional groups will be described. We have discovered a series of sulfur-bridged anthracenes which undergo a unique photochemical extrusion of sulfur monoxide (SO) to give an emissive pi-conjugated dianthracene product. Applications of this novel photoreaction in fluorescent photopatterning and fabrication of anti-counterfeiting security patches will be discussed.

Prof. Muralee Murugesu
University of Ottawa

Dynamic guest adsorption visualized through crystal free crystallography

Metal–Organic Frameworks continues to fascinate researchers not only owing to their aesthetic beauty but also to their immense potential application ranging from gas adsorption to catalysis. Recently, the use of MOFs as crystalline sponges for crystal-free crystallography has attracted much attention as these systems enable crystallography on molecules that are hard to crystallize. Moreover, through single-crystal X-ray crystallography, the binding of a guest that displays a variety of binding motifs in the site of adsorption can be directly observed. As such confinement effects and host guest interacting can be probed and employed towards the design of the next generation of high performing MOFs. In this presentation, we provide a series of examples that demonstrate the power of this crystal-free crystallography technique; which is on the verge of revolutionizing single-crystal X-ray crystallography.

Prof. Ngong Kodiah Beyeh
Oakland University

Self-Assembly of Biohybrid Materials with Macrocyclic Receptors

Multivalency is a very important concept in supramolecular and biochemistry. Multivalent interactions are ubiquitous throughout nature and are used to create novel materials with specific properties and functions.[1] Synthetic materials that interact with biological target molecules are of paramount importance for the development of various biotechnological applications.[2] Herein, we present the design, formation and host-guest properties of biohybrid assemblies between two groups of cationic macrocyclic receptors (resorcinarenes and pillar[5]arenes) and two biomolecules (apoferritin protein and heparin sugar).[3]

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Dr. Nicholas Vukotic
PROTO, University of Windsor

From Academia to Industry to Synergy

The path from academia to the world of industry can be complex, as one begins to traverse an unknown landscape with new challenges and self-doubt around every corner. However, the reality is that academia and industry have much more in common than you would first think. In this presentation, I will highlight a portion of my journey through this landscape and the tools I found useful during this transition. These tools eventually lead me to a synergistic way of combining my academic experience in material science with my industrial experience with X-ray diffraction instrumentation.

Dr. Ronald Rubinovitz
Thermo Fisher Scientific

The Use of FTIR in the Characterization of Crystal Structures

Fourier Transform infrared spectroscopy (FTIR) offers the benefit of providing functional group molecular bond information and as a result is a well-established analytical technique that is utilized in many distinctive fields, including the characterization of crystal structures. However, the use of FTIR requires selection of the optimal sampling configuration relative to sample type since the correct technique often makes a dramatic difference in spectral quality. Various sampling configuration modes are customarily used, such as transmission, attenuated total reflectance (ATR), specular reflectance as well as diffuse reflectance. This presentation will review investigations of a variety of crystal types such as pharmaceutical polymorphs and cocrystals, as well as metal–organic frameworks with emphasis on the applicability of each sampling technique as well as examples of the insight into molecular structure and interactions that FTIR provides.

Prof. Sally Brooker
University of Otago

Spin Crossover

Spin crossover (SCO) occurs only in complexes of metal ions in appropriate d electron configurations, and only when an appropriate intermediate ligand field strength is imposed on them.[1] Switching can be induced by application of a variety of stimuli, most commonly change in temperature, but also by change of pressure, light irradiation, application of an electric or magnetic field, or by the presence/absence of a guest. The last of these is of particular interest with regard to the development of guest sensors. For some systems, thermal hysteresis loops are observed: these are of considerable interest for memory applications, for which the lifetime of the sample in the meta stable state is of key importance.

Gaining predictability of field strength, and hence SCO, is also highly desirable, but remains a considerable challenge. This issue is being intensively probed by a number of groups internationally, with some significant breakthroughs reported recently, in the solid state and in the solution phase.

This lecture will start with an introduction to spin crossover,[2] then present our own efforts, ranging from the observation of unusual scan rate dependence of thermal hysteresis loops, to pressure-induced SCO, to tuning of switching temperature, the development of SCO-based sensors, and finally to a method enabling easy prediction of spin state in solution, in advance of synthesis,[3] for two quite different families.

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Abstracts of Contributed Talks

The contributed talks are held in room SP S110

Alex Mayo
Solid State Pharma Inc.

Improving Experimental Success of Co-Crystallization with Computational Pre-Screening of Co-Formers

Authors:
Xibo Feng, Alastair Price, Erin Johnson, R. Alex Mayo, Rishi Venugopal, Lauren MacEachern

Discovery of pharmaceutical co-crystals is crucial to improving the bioavailability of poorly soluble drugs and protecting and extending patents for the drug developer. Unlike salt formation, co-crystallization is harder to predict as there is no formal ionization of the drug and counter-ion. Because of the uncertainty in choosing successful co-formers, experimental screening for co-crystals can be a costly endeavour with low success rates. Over the past decade, progress has been made in using quantum-chemical calculations to better understand co-crystals, and to predict successful co-formers prior to experimental work. Significant success can be achieved with much shorter computational time requirements by calculating the binding affinity between the co-former and drug molecule rather than full crystal structure predictions. The development and use of a computational method to determine and rank the binding energies of hetero-dimers in the gas phase in order to generate a co-former list that is top-heavy in hits prior to experimental screening will be described. Benchmarking of the method with literature data sets will also be discussed.

Austin Peach
University of Windsor

What Can Multi-Component Milling Tell Us About Fluoxetine HCl Cocrystals?

Authors:
Austin A. Peach, Sean T. Holmes, Michelle T. Quan, and Robert W. Schurko*

The solid forms of active pharmaceutical ingredients (APIs), such as polymorphs, pseudopolymorphs, and amorphous solid dispersions, have unique properties such as stability and solubility that can affect their bioavaibility and shelf life. These properties are dependent on the molecular-level structure of the solid form of the API; as such, they can be modified or tuned with targeted synthetic or preparative procedures. Cocrystalline forms of APIs, which feature the API and a pharmaceutically acceptable coformer, have garnered much attention, since they provide a wider array of potentially stable and bioavailable solid API forms in comparison to the pure, bulk API. They are commonly produced by both solvothermal and mechanochemical methods; however, mechanisms of cocrystallization by mechanochemical methods remain poorly understood.

Multi-component milling (MCM), which is the focus of the present work, has been employed by Fischer et al. to understand cocrystillization of APIs under mechanochemical conditions.[1,2] MCM involves two types of milling experiments: (i) competitive milling and (ii) stability milling. Competitive milling involves milling physical mixtures of the API and potential coformer(s), whereas stability milling uses a cocrystal and a different coformer as the reagents. Fluoxetine HCl (Fluox), the API in the antidepressant Prozac®, forms stable cocrystals with three carboxylic acid coformers: benzoic acid, fumaric acid, and succinic acid.[3] We have previously demonstrated that their mechanochemical preparations are superior to solvothermal methods, in terms of both the synthetic yields and reaction timeframes.[4] However, structurally similar coformers, such as malonic acid, glutaric acid, and adipic acid, do not cocrystallize with Fluox under similar experimental conditions. Thus, we propose the use of MCM to garner insight into the formation of Fluox cocrystals.

Herein, the use of competitive milling and stability milling for understanding the formation of Fluox cocrystals are presented. First, the liquid-assisted grinding syntheses of fluoxetine HCl cocrystals using both types of milling are discussed. Second, the ^{35}Cl SSNMR experiments that are used in tandem with powder X-ray diffraction (PXRD) to characterize the products of the MCM syntheses that are described. Because fumaric acid and succinic acid cocrystals have very similar PXRD patterns, it is difficult to differentiate them by PXRD alone; however, each cocrystal has a unique Cl– environment with a distinct local hydrogen bonding network, and therefore, a distinct set of ^{35}Cl electric field gradient (EFG) tensor parameters can be used to determine the cocrystal identity based on the second-order quadrupolar pattern observed in the ^{35}Cl SSNMR spectra. Lastly, coformers are ranked based on their ability to form cocrystals with Fluox; this leads us to explore the idea of solid-state extraction for the formation of increasingly complex and novel cocrystals.

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Colum O’Connor
Center for Defence Chemistry, Cranfield University

Co-crystals: Designer explosives for the future

Authors:
Colum O'Connor, Philip P. Gill, Ranko Vrcelj, Kyle Ramos, Gary K. Windler

Co-crystallization provides a means for forming new crystal structures from existing explosive molecules and thus modifying physical properties relative to the pure constituents. Properties such as impact sensitivity, thermal behaviour, and detonation performance that depend upon crystal structure and/or composition can be modified. A systematic study of the formation of co-crystals with N-heterocycles containing conjugated π-systems. Mechanochemical techniques coupled with solvent evaporation and theoretical modelling, have been adopted to explore potential for co-crystallization. A series of amine containing conjugated 5-membered heterocycles were combined with 2-naphthol as a co-former, wherein the presence of functional groups and number of heteroatoms on the heterocycles were modified. The impact on bonding position and capability has been assessed to develop rules for co-crystallisation of this class of material. This talk will examine the successful and unsuccessful co-crystallization experiments and propose some initial predictions of rules for co-crystallization of inert and explosive heterocyclic molecules.

Protocols for the synthesis of co-crystals using mechanochemical techniques will be proposed. These have been developed to aid screening studies to maximise potential of identifying co-crystals.

Dominique Leckie
University of Windsor

Transition Metal Complexes of the 1,3,2-Dithiazolyl Radical

Authors:
Dominique M. Leckie, Javier Campo, and Dr. Jeremy M. Rawson

The field of single molecule magnets has provided access to systems in which individual bits of data can be stored at the molecular (nm and sub-nm) scale. Here the energy barrier to reversal of the magnetization is given by DS2 where D reflects the magnetic anisotropy and S is the spin ground state of the complex. Most SMMs are based on 3d or 4f metal ions as a source of both D and S but the use of paramagnetic ligands (the so-called "metal/radical approach") has attracted attention to increase the spin ground state in polynuclear complexes.

Extensive work by Preuss has investigated both 3d and 4f metal complexes of dithiadiazolyl radicals.[1] The related dithiazolyl radicals have been poorly studied in comparison.[2] Here, we present the synthesis and characterization of a series of mononuclear complexes of 4-methyl-benzo-1,3,2-dithiazolyl, MBDTA, with $M(hfac)_2$ (M = Mn, Co, Ni, Cu, Zn) using X-ray diffraction, EPR spectroscopy and SQUID magnetometry.

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Hatem M. Titi
McGill University

Greener hypergolic solid fuels for aerospace application

Authors:
Hatem M. Titi, Joseph M. Marrett, Mihails Arhangelskis, Gandrath Dayaker, Robin D. Rogers and Tomislav Friščić

This presentation will outline new approaches to obtain cleaner, safer and inexpensive hypergolic fuels,[1] i.e. materials that spontaneously ignite in contact with an oxidizer. Such hypergols are critical components of high-energy propulsion systems required in aerospace applications. The aerospace industry, however, is facing a major environmental and health challenge due to its dependence on hydrazine-based hypergols which combine high energetic value with, unfortunately, highly toxic and extremely cancerogenic hydrazine-based molecules.[2] In order to help resolve this conundrum of aerospace propulsion technologies, we present the very first strategies that promote hypergolicity through simple kits provided by crystal engineering via covalent and non-covalent bond modifications of known materials. These structural manipulations of the presented strategies enable access to materials which are significantly safer to handle than hydrazine hypergols, while maintaining high combustion energies and ultrafast ignition delays as low as 2 ms.[3]

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Igor Huskić
McGill University

Proton Conductivity and Polymorphism in Organic Minerals and Their Analogues

Authors:
Igor Huskić, Lim Dae-Woon, Novendra Novendra, Hatem Titi, Filip Topić, Alexandra Navrotsky, Igor Pekov, Sergey Krivovichev, Hiroshi Kitagawa, Tomislav Friščić

Organic minerals are a class of naturally occurring solid materials that incorporate organic carbon in their composition. These materials exhibit structural and functional similarities with modern advanced synthetic materials.[1] For example, humboldtine, the iron(II) oxalate dihydrate mineral exhibits proton conduction properties comparable to designed synthetic materials.[2] Stepanovite and zhemchuzhnikovite are two oxalate-based minerals discovered mid 20th century and recently reported as first known examples of naturally occurring metal–organic frameworks.[3] Analogues of these minerals have been explored for their magnetic and optical properties.[4]

Herein, we explore the proton conductivity properties of stepanovite and zhemchuzhnikovite, as well as a synthetic polymorph of stepanovite. Small structural differences between the two stepanovite polymorphs result in a ten-fold increase of proton conductivity values. Additionally, reversible dehydration/rehydration process is demonstrated using in situ methods. The materials exhibit high thermodynamic stability, with a pronounced stabilizing effect of substituting aluminium for iron, illustrating a simple design to access highly proton-conductive MOFs without using complex organic ligands. The potential for polymorphism in these compounds and their structural analogues have also been explored.

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Ivana Brekalo
Georgetown University

Are guanidinium sulfonates formally microporous

Authors:
Ivana Brekalo, David Deliz, Leonard J. Barbour, Michael D. Ward, Tomislav Friščić, K. Travis Holman

With the recent emphasis on the importance of porous materials, so called porous hydrogen bonded organic frameworks (HOFs)[1] have started gaining attention. A well-known class of HOFs are bisguanidinium organodisulfonates (GS). GS have been extensively explored for the last 20 years due to their diverse host-guest chemistry, as well as their inclination towards architectural isomerism, a phenomenon in which a material can have the same composition and the same supramolecular bonding motive, but still differ in the overall crystal structure due to topological differences.[2] Especially interesting is the persistence of the 2D hydrogen bonded sheet motif, which is so reliable that it can allow for targeted synthesis of a multitude of different pillared architectures, such as the bilayer or brick structure, where the type of architecture depends on the size of the guest and the pillar type. Most importantly, these materials have been shown to exchange guest molecules in a single crystal-to-single crystal fashion.[3]

Surprisingly, despite the stability of these frameworks, the desolvation of GS has not been extensively studied, and the structures of their empty forms-either 'collapsed' or 'open/porous'-have gone unreported. As a result, despite 20 years of prominence in the crystal engineering community, the formal existence of microporosity in the GS class of compounds has not yet been established.

In this work we study the desolvation of guanidinium organodisulfonate materials and demonstrate that they are formally microporous. Furthermore, we study the absorption of gases into these materials via Single Crystal-to-Single Crystal transformations.

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Jennifer Murphy
Memorial University of Newfoundland

How calcite 'musseled' its way into supercapacitors

Authors:
Jennifer N. Murphy, Kelly Hawboldt, Doug R. MacFarlane and Francesca M. Kerton

Green chemistry has played a key role in the field of renewable feedstocks, an area of research that has been increasing rapidly over the last 15 years. Memorial University has been leading the way in the search for ocean-based renewable feedstocks.[1] Aquaculture operations are increasing all over the world to meet global demands for protein. Since 2011, mussel farming has grown by 47% in NL and continued growth will lead to waste disposal problems. Mussel shells are a renewable source of $CaCO_3$, a widely used inorganic material that is mined from the Earth’s crust, and the residual protein on the mussel shells are rich in amino acids that could be used in nutraceuticals and fish feeds.

Having already developed a shell cleaning protocol using environmentally-friendly and easily implemented technologies[2] and fully characterized the shells after heat treatment to yield various calcium carbonate materials, this talk will highlight the discovery of a unique calcite material made from waste mussel shells. The synthesis of our unique calcite will be described as well as its use as inorganic filler in ionic liquid gel polymer electrolytes (ILGPEs) for supercapacitors. The addition of 2 wt.% calcite increased the mechanical stability of ILGPEs and decreased costs by 17%. Additionally, supercapacitors fabricated with calcite containing electrolytes had a higher power density, stability and lifetime. This research is promising for the development of safe, solid-state electrolytes for supercapacitors.

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Juby Varghese
Clarkson University

Metal–Organic Frameworks as Platforms for the Nanostructuration of Single Molecule Magnets: New Insights from HRTEM

Next-generation computer technologies require ultrahigh-density data storage devices and quantum computing based on isolated spin-carriers, so-called molecular spintronics. Single-molecule magnets (SMMs) show great potential for such applications due to their unique magnetic properties. Their magnetic bistability allows switching from total spin up to total spin down on a molecular level where each molecule serves as a magnetic bit of information. The quest for the design of new SMMs with improved properties is ongoing, however, coupling of the nanoscale units to the macroscopic world remains a major challenge. Practical applications of SMMs require their organization in 2D or 3D networks while being in a protected environment to enable read-and-write processes. Metal–organic frameworks (MOFs), due to their porous nature and tunability, are excellent candidates to overcome this challenge. This work is the first systematic investigation exploring MOFs as platforms for the controlled nanostructuration of molecular magnets in both bulk polycrystalline powder and thin film forms. Subsequent characterization of SMM@MOF composites using HRTEM provides previously inaccessible visual structural insights into these nanomagnetic composites bringing us one step closer to the development of spintronic devices combining functional properties of both SMMs and MOFs.

Lana Hiscock
Wilfrid Laurier University

Synthesis, Characterisation, and Photophysical Properties of a Series of 6,13-Dicyanoheteropentacene Analogues

Authors:
Lana Hiscock, Louise Dawe, Kenneth Maly

The synthesis of novel materials for organic electronics is a growing field with potential end applications in energy storage, energy harvesting, displays, and more. Probing the characteristics and properties of novel aromatic and heteroaromatic structures, which increasingly appear in these devices, is a worthwhile pursuit through which we gain insight into the structure-function relationship of previously unknown substances. This in turn allows for more precise tuning of properties for future materials. In certain cases, intermolecular interactions can lead to interesting (and useful) properties such as aggregation-enhanced emission (AEE). Utilizing new materials in novel applications, however, requires a full understanding of their chemical behavior and characteristics.

Recent work within our group has led to the reported synthesis of substituted 6,13-dicyanotetraoxapentacene (DCTOP) analogues prepared by the nucleophilic aromatic substitution (SNAr) of tetrafluoroterephthalonitrile (TFTP) with catechol derivatives.[1]

We have now extended this SNAr methodology in order to prepare a series of novel dicyanoheteropentacene analogues incorporating oxygen, nitrogen, and/or sulfur into the linear polycyclic core. Compared to the tetraoxa congeners, these new derivatives likewise display intense luminescence in both solution and solid states, in addition to brilliant dye-like colouration (yellow to red). The synthesis, photophysical and mesomorphic properties, and the solid-state organization of these compounds will be described.

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Lara Watanabe
University of Windsor

Investigation between the mononuclear and dinuclear transformation of cobalt dithiolates

Authors:
L. K. Watanabe, J. M. Rawson and C. L. B. Macdonald

Metal dithiolene complexes exhibit intense colors, multiple oxidation states, reversible redox reactions and the ability to take on different geometric conformations, making them ideal in a variety of materials applications. To date, many dithiolate complexes contain strongly electron-withdrawing groups, such as $(NC)_2C_2S_2^{2-}$ and $(F_3C)_2C_2S_2^{2-}$, while the pi-conjugated dithiolates contain commercial benzenedithiolate or toluene dithiolate ligands. More recently, it has been shown that alkoxy-functionalized bis(benzo)-1,2,5,6-tetrathiocins are able to undergo oxidative addition to low valent group 10 metal complexes (Ni, Pd, Pt). This presentation extends the reactivity to the group 9 complex $CpCo(CO)_2$ with tetrathiocins. Reaction of cyclopentadienylcobalt dicarbonyl with the respective dialkoxy-functionalized bis(benzo)-1,2,5,6-tetrathiocins under microwave conditions generated the mononuclear or dinuclear complexes $[CpCoL]_{n\ (1\ -\ 2)}$. These complexes were characterized by single crystal and powder X-ray diffraction, NMR spectroscopy and FT-IR. Thermal and mechanochemical transformations between 16e- monomer and 18e- dimer are discussed.

Novendra Novendra
University of California, Davis

Experimental Evaluation of Substitution Effect on Thermodynamic Stability of Zeolitic Imidazolate Frameworks

Authors:
Novendra Novendra, Mihails Arhangelskis, Athanassios D. Katsenis, Tomislav Friščić, Alexandra Navrotsky

Zeolitic imidazolate frameworks (ZIFs) are a class of metal–organic frameworks (MOFs) having isomorphic topology with zeolites and are composed of tetrahedrally coordinated divalent metals, such as Zn or Co, interconnected by imidazolates linker. This family of material has a wide array of applications, such as catalyst, gas separation, energy storage, and other applications due to its versatile chemical compositions[1,2]. The wide array of possible ZIF compositions begs the question on how the composition, especially the substitution on the imidazolate linker would affect the thermodynamic stability of the resulting ZIFs. In this study, fluorinated ZIFs ($Zn(CF_3Im)$) was shown to be thermodynamically accessible by theoretical prediction and was successfully synthesized with mechanochemical synthesis. Two different polymorphs (qtz and SOD) that was successfully synthesized were analyzed with room temperature acid solution calorimetry to measure their solution enthalpy and calculate their enthalpy of formation from ZnO and the corresponding imidazoles. The enthalpy of formations was obtained to be exothermic, indicating thermodynamically driven formation. Additionally, by comparing the enthalpy with previously studied Zn(MeIm) and Zn(EtIm), strong effect of framework topology, framework density and substitution on the stability was observed.
To further understand the sole effect of substitution on the thermodynamic stability, additional isostructural ZIFs with open SOD topology were prepared with different substitutions on the 2-position of the imidazolate ligand (Cl, Br, I, vinyl, and ethynyl). Again, here it was observed that the enthalpy of formation was all exothermic, indicating thermodynamically driven formation. Methyl substitution stabilizes the structure the most, while CF_3 substitution destabilizes the structure. The main contribution to this exothermic effect is the change in zinc local bonding (from oxygen to nitrogen), while the formation of the framework and the porous structure itself is endothermic[3]. The results also exhibit a correlation between the measured thermodynamic stability and molar volumes, where the enthalpy of formation becomes more endothermic with increasing molar volume. This trend is similar to that seen before in other porous systems, including zeolites, mesoporous silicas, and other MOFs[4].

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Sean Holmes
University of Windsor

NMR crystallography of active pharmaceutical ingredients and nutraceuticals: Insights into crystal structure from dispersion-corrected DFT calculations

Authors:
Sean T. Holmes and Robert W. Schurko

^{35}Cl solid-state NMR (SSNMR) spectroscopy has emerged as a valuable method for characterizing the molecular-level structures of HCl salts of organic molecules. Interest in this field has been spurred by the ubiquity of chloride anions among active pharmaceutical ingredients (APIs) and nutraceuticals, which are prepared and stabilized as HCl salts, both in bulk materials and formulations. ^{35}Cl SSNMR is able to provide distinct spectral fingerprints for HCl APIs and their polymorphs, solvates, hydrates, and cocrystals because of the strong dependence of the ^{35}Cl electric field gradient (EFG) on the local structural environment; in particular, ^{35}Cl SSNMR can provide key insights into the arrangements of hydrogen atoms participating in $H \cdots Cl$ hydrogen bonds. Conventional density functional theory (DFT) calculations have not been effective for modeling the local environments of chloride anions; this limitation was overcome by using a dispersion-corrected DFT method developed by our group for refining crystal structures. The dispersion force fields used in these calculations have been parameterized such that calculations on the energy-minimized structures yield accurate predictions of the ^{35}Cl EFG tensor parameters (as well as the EFG tensors of other nuclides, including ^{14}N, ^{17}O, ^{23}Na, etc.). The EFG tensor parameters calculated using these refined structures are superior to those of comparable values obtained from calculations on structures derived from neutron diffraction. Furthermore, this refinement strategy is facile to implement in many plane-wave DFT codes. This talk will also discuss application of ^{35}Cl SSNMR to (i) refine structural features of materials that have been characterized through diffraction methods, and (ii) derive the crystal structures of systems in the absence of high-quality diffraction data.

Shefa Alomari
Clarkson University

Design and Synthesis of Zwitterionic Metal–Organic Frameworks

Authors:
Shefa Alomari, Dr. Mario Wriedt

Metal–organic frameworks (MOFs) have emerged as a new type of porous material. Their crystalline structures are composed of metal clusters connected by polytypic organic linkers. The characteristics of the metal and organic ligand blocks are important for controlling the resulting topologies, pore environments, and functionalities and hence affect the characteristics of the MOFs to capture specific guest molecules. As a new means to introduce charged-polarized porosity into MOFs we explore zwitterionic (ZW) ligands as MOF building blocks. These ligands are composed of both cationic and anionic functional groups resulting in an electrostatic field gradient on their molecular surfaces. Incorporating them into MOFs leads to polarization effects on guest molecules, resulting in enhanced adsorption enthalpies and multi-stimulus-responsive properties. N-substituted pyridines, namely pyridiniums, and their derivatives are among the most famous zwitterions, however, the design and synthesis of new pyridinium-based ligands are challenging. In this research, I explore the synthesis of new rigid zwitterionic ligands through multi-non-standard organic protocols. In this talk, I will present on the crystal structures and physical properties of new ZW MOFs. I will show that these systematic investigations will pave the way to develop new functional materials with improved adsorption properties.

Sina Mirzaeifard
McGill University

Simulation and Modeling of the Interface between the Liquid Water and Methane Hydrate Crystal

Authors:
Sina Mirzaeifard, Phillip Servio, Alejandro D. Rey

The methane hydrate and liquid water phases coexist in a variety of industries such as petroleum and gas. The liquid-crystal interface plays a vital role in mass transfer across the phases. In this work, we use powerful molecular dynamics technique to study the system of water and crystalline methane hydrate. We state that the mechanical definition with use of the unique NPAT ensemble and slab length of the crystal lattice parameter can compute the interfacial energy of a non-planar interface. In addition, we manipulate the equation related to the surface tension to include the surface deformation. In a specific range of temperature and pressure, we show that the interfacial tension increases with increasing temperature or decreasing pressure due to less surface entropy and scattered molecular distribution. We calculate the excess stress and enthalpy, pair radial distribution function, local density profile, hydrogen bond density, and polar charge distribution to fully characterize the system in molecular scale, and subsequently, confirm the interfacial tension effect in the gas hydrate formation.

Zineb Ras Ali
Brock University

Synthesis and magneto-structural studies of 4f complexes of dibenzo15C5 macrocycles

Authors:
Z. Ras Ali, M. Pilkington

Although crown ether macrocycles are widely utilized in many fields of chemistry, their applications as ligands for the assembly of single-molecule magnets (SMMs) has only recently been explored. In this respect, our group has been exploring the structure-directing capabilities of crown ether macrocycles together with 4f ions for the discovery of stable SMMs with high coordination numbers and a strong axial ligand field. The cavity sizes of smaller crowns such as 15C5 and 12C4 afford ‘half-sandwich’ topologies, where the metal ions are axially coordinated out of the plane of the crown and axial solvent molecules and/or anions complete the coordination geometries.[1,2] In order to investigate further how subtle modifications to the organic framework of crown ether macrocycles effects their structure-directing properties, the synthesis, structure and magnetic properties of 4f complexes of dibenzo15C5 will be presented.

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Abstracts of Poster Presentations

The poster presentation sessions are held in the RF Center

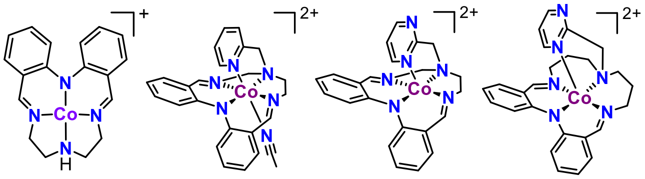
Abdullah Abudayyeh
University of Otago

Visible Light–Driven Reduction of H^+ or CO_2 Catalysed by Cobalt Macrocycles

Authors: Abdullah M. Abudayyeh, Fola Akogun, Olivier Schott, Garry Hanan* and Sally Brooker*

Growing concerns about the depletion of oil reserves, endless emission of CO_2, and associated anthropogenic climate change, have initiated great international interest in carbon-neutral fuels as well as CO_2 capture/utilisation.[1] Due to its potential to be *carbon-zero* when generated using renewable energy, *hydrogen* can be regarded as the greenest possible fuel: it has the greatest energy density and generates energy without the production of greenhouse gases. An alternative scenario is to *reduce CO_2* to form *carbon-neutral fuels* and other value-added chemicals.[2] Despite much effort over recent decades, to date attempts to devise an inexpensive system either for hydrogen production (HER) or CO_2 reduction (CO2RR), driven by light energy, on a large scale, are still hampered by significant academic and engineering obstacles.

We recently reported that the $[Co^{II}\mathbf{L}^{Et}](BF_4)\cdot H_2O$ complex (Figure, left)[3] of a Schiff base macrocycle derived from 2,2'-iminobisbenzaldehyde[4] was the most active catalyst, 3x greater than the literature standard $[Co^{III}(dmgH)_2(py)Cl]$, of the 17 cobalt complexes we tested for photocatalytic hydrogen production.[5] This presentation will describe the subsequent development of a family of cobalt complexes closely related to this lead complex, and their photocatalytic performance for both HER and CO2RR, as we look for improvements in activity and for useful structure-function relationships.



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Adriana Danko
Concordia University

Stability of Zr-UiO-66 Metal–Organic Frameworks in Aqueous Environments under Varying pH Conditions

Authors: Adriana Danko, Ashlee J. Howarth*

Metal–organic frameworks (MOFs) are porous materials that are widely used for many applications ranging from carbon dioxide (CO_2) capture and storage to the extraction of analytes from food matrices. These impressive hybrid materials are synthesized by combining metal nodes with organic linkers to form lattices. Their framework and pore size characteristics can be tuned and vary amongst the different metals, linkers and reaction conditions used. Of all the existing MOFs, Zr-UiO-66 is reported to be among the most stable. Rare earth MOFs are a relative new class of MOFs, and not as much is known about their stability. In attempt to understand more, the aqueous phase stability of rare earth MOFs are compared to zirconium based-MOFs and the materials are characterized using powder X-ray diffraction (PXRD) and nitrogen adsorption analysis.

Alicia McTaggart
Concordia University

The role of pH in the growth of silica-carbonate microstructures

Authors: Alicia McTaggart, Dr. Wim Noorduin and Lukas Helmbrecht (AMOLF, Netherlands), Dr. Louis A. Cuccia*

Spurred by lessons learnt from the ability of nature to “design” biominerals with a high degree of control over their shape, size, mineral phase and hierarchical assemble over multiple length scales, a multitude of bottom-up research strategies have been geared towards developing self-assembled inorganic materials having superior functionality and complexity. Of particular interest are 3D nano-crystalline composite materials, characterized by long-range orientational order and highly curved surfaces, which can be synthesized from the coupled precipitation of the carbonates of barium, strontium and aragonite-type calcium carbonate with silica in alkaline (pH ~10-11.9) environments under the influence of atmospheric CO_2. These silica-carbonate microstructures include cardioidal sheets, helicoids, “worms”, flower-like and globular structures. In this work, we aim to show the importance of the role of pH in the assembly and growth of silica-carbonate microstructures. These microstructures will be grown by utilizing the principles devised by Noorduin et al. under additive-free conditions. We will then investigate how the growth characteristics of silica-carbonate microstructures can be tuned as a function of concentration of sulphonated azo dye and pH regulation in the precipitation reactions. Indeed, this research also provides indirect evidence for accelerated growth rates of the microstructures from solutions containing dye as implied by an increase in size relative to control experiments without dye during a growth period of 1.5-2 hours. Directed strategies to control both shape and size are of fundamental importance since it is well-known that the chemical composition and physical properties of a material are intimately connected to its function. Light and scanning electron microscopy (SEM) are the principle tools used for the characterization of the as-formed microstructures.

Blaine Fiss
McGill University

Mechanochemical Phosphorylation of Polymers and Synthesis of Flame-Retardant Cellulose Nanocrystals

Authors: Blaine G. Fiss, Lucius Hatherly, Robin S. Stein, Tomislav Friščić*, Audrey Moores*

Flame-retardant materials are used extensively in areas ranging from general construction and textiles to the aerospace and automotive industries. Typically, these industries employ halogenated organic molecules or inorganic phosphates as flame-retardant materials. However, the toxicity of these materials, both to the environment and human health, has become a topic of greater concern. New flame-retardants are needed which are both effective at preventing the ignition and propagation of fire, while being environmentally benign, both in their manufacture, design and usage. Herein we describe a new, environmentally-friendly solvent-free mechanochemical synthesis of both covalently phosphorylated polymers and cellulose nanocrystals as greener alternatives to traditional flame-retardant materials.[1] Thermal analysis and ^{31}P magic angle spinning NMR spectroscopy were used to determine the thermal stability and extent of phosphorylation of the resulting material, revealing unprecedented phosphate loadings, averaging to ca. 3,300 mmol/kg, compared to 1,600 mmol/kg found in previous literature. This solvent-free methodology, which uses phosphorus(V) oxide as simple, inexpensive and solid phosphorylation agent, was successfully applied also to synthetic and biological polymers, such as poly(vinyl alcohol) and lignin. Preliminary tests confirm the feasibility of resulting phosphorylated materials as protective coatings on wood substrates.

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Cameron Lennox
McGill University

Ultralight main-group imidazolate frameworks

Authors: Cameron Lennox, Joshua Crew, Jean-Louis Do, Ashlee J. Howarth, Omar K. Farha, and Tomislav Friščić*

Metal–organic frameworks (MOFs) have been established as a tunable and porous materials, whose synthesis remains challenging in terms of efficiency and environmental impact.[1] One class of such material that has been particularly poorly explored are boron imidazolate frameworks (BIFs),[2] main group analogues of the popular class of MOFs known as zeolitic imidazole frameworks. The general design for such materials relies on replacing the divalent tetrahedrally-coordinated metal nodes, typically zinc or Co(II), with alternating lithium cations and tetrakis(imidazolato)borate anions. These replacements make the resulting BIFs particularly attractive as a lightweight, microporous material. The synthesis of BIFs has, however, been challenging due to the use of harsh solvothermal synthetic conditions that can readily lead to framework re-arrangement into a non-porous material. We present efforts in the development of solvent-free mechanochemical routes for the assembly of a wide range of BIF materials, providing a simultaneously cleaner and faster access to such frameworks.[3]

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Cameron Vojvodin
University of Windsor

NMR Crystallography of Multi-Component Crystals Containing Urea

Authors: C.S. Vojvodin, D.A. Hirsh, S.T. Holmes, I. Huskic, T. Friščić, and R.W. Schurko

The rational design of single-phase multi-component crystals (MCCs) is a flourishing area in crystal engineering which encompasses a variety of different compositions such as solvates, salts and cocrystals. MCCs are of particular interest to the pharmaceutical industry as they can be made from an active pharmaceutical ingredient (API) and one or more pharmaceutically acceptable coformers. By carefully selecting the appropriate constituents and mode of preparation, it is sometimes possible to tailor the physicochemical properties of the crystalline solid to have better solubility, stability, bioavailability and/or shelf-life.[1,2] Two common methods of synthesizing MCCs are slow evaporation and mechanochemistry; of these, the latter has been less explored. The mechanochemical method of liquid-assisted grinding (LAG) incorporates all modern tenets of “green chemistry” (i.e., it requires little solvent, low energy input, and no harsh reagents or waste).[3] There is great interest in the syntheses of cocrystals containing active pharmaceutical ingredients (APIs), predominantly for the production of stable dosage formulations; however, there are few reports describing their rational design or the reaction mechanisms underlying their formation.[4,5] Powder X-ray diffraction (pXRD) and solid-state NMR (SSNMR) spectroscopy are well suited for studying the formation of MCCs, both allowing for the identification and characterization of distinct crystalline phases and the detection of impurities. Most importantly, SSNMR is extremely sensitive to local structure differences that result from unique hydrogen bonding networks in different solids. Thus, careful characterization of these materials by SSNMR provides an avenue for structural solution, and aids in the development of NMR crystallography protocols that can be applied to a diversity of solids.[6-8]

Here, we present an NMR crystallographic investigation of MCCs of the form MCl:Urea:xH2O (M = Li, Na, Cs; x = 0, 1, 2) made by mechanochemical syntheses; this includes characterization by multinuclear (^{35}Cl, ^{23}Na, ^{7}Li, and ^{133}Cs) SSNMR spectroscopy, synchrotron XRD, and thermogravimetric analysis. The study of these model systems using plane-wave density functional theory calculations[9] and Rietveld refinement of synchrotron XRD data aid in understanding how these MCCs form; this could lead to the development of MCCs and cocrystals of significantly more complex systems, including those involving APIs.

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Carmen Yan
Concordia University

Zirconium and Yttrium mixed-metal–organic frameworks

Authors: Carmen Yan, Hatem Titi, Ashlee Howarth*

Metal–organic frameworks (MOFs) are crystalline porous materials that consist of metal clusters that are joined together with organic linkers. The versatile structures of MOFs, makes them ideal materials for use in applications such as gas storage, catalysis, and as green alternatives for wastewater remediation. Zr- based MOFs are usually known in literature for their robust nature and utility in a variety of applications. Rare earth MOFs belong to a relatively new class of MOFs and not much is known about their stability or intricate structural features. This research focuses on the synthesis of Zr and Y MOFs, as well as mixed-metal derivatives. The comparison of pure versus mixed-metal MOFs can provide an insight of the different coordination environments of Y(III) and Zr(IV) as well as the differences in catalytic activity or adsorption properties.

Chris Copeman
Concordia University

Carbonate Loaded MOF-808 for Wastewater Remediation

Authors: Chris Copeman, Ashlee J. Howarth*

Metal–Organic Frameworks (MOFs) are coordination polymers consisting of metal centers connected to one another by organic ligands to form crystalline networks that are often highly porous. Due to the vast array of metal and organic linker combinations, and a multitude of topologies, metal–organic frameworks have been investigated for a variety of uses such as catalysis, gas separation and storage, as well as air pollution and wastewater remediation. MOF-808 ($Zr_6O_4(OH)_4(HCOO)_6(BTC)_2$) is a robust, water stable metal–organic framework with high surface area well suited for wastewater treatment and remediation. This work focuses on the removal and replacement of the formate ($HCOO^-$) ligands with carbonate (CO_3^{2-}) ligands. When placed in an acidic solution, the carbonate can be released and becomes protonated to neutralize acidic solutions without introducing additional cations (Na^+, Ca^{2+}, K^+, etc.) while simultaneously leaving a vacancy on the metal node for further adsorption of unwanted species.

Daniel Therien
McGill University

Mechanoenzymatic breakdown of chitin into N-acetylglucosamine in the absence of bulk solvent

Authors: J.P. Daniel Therien, Fabien Hammerer, Tomislav Friščić, and Karine Auclair

It is estimated that 6-8 million tons of crustacean shell waste is generated annually worldwide, with most of it being discarded into landfills or back into the ocean. Chitin is one of the major components of crustacean shells and is the most abundant nitrogen-containing biopolymer found on Earth, consisting of repeating β-(1,4)-N-acetylglucosamine (GlcNAc) units.[1] Given that crustacean shells are a renewable biological feedstock, research into transforming this waste into industrially relevant molecules has been gaining traction. For example, the ability to transform GlcNAc into nitrogen-containing furans has been reported.[2,3] However, current methods to obtain GlcNAc from chitinous biomass typically employ harsh, aggressive chemicals (such as concentrated HCl or NaOH) at high temperatures and therefore lack sustainability. In contrast to the chemical route, enzymatic catalysis provides a significantly milder approach. Enzymes capable of hydrolysing chitin, called chitinases, are produced across living organisms, from humans to bacteria and fungi. Unfortunately, the current enzymatic methods to hydrolyze chitin typically rely on large volumes of solvent, and harsh pre-treatments of the chitin substrate to aid in suspending the insoluble material in water.[4,5] Our group has recently reported that some enzymes can be more efficient when used in the absence of bulk aqueous or organic solvent.[6] This is possible thanks to a combination of ball milling and accelerated aging (static incubation) repeated over several cycles, which we call reactive aging (RAging). This approach has allowed us to efficiently digest cellulose and plant biomass without the need for harsh chemicals or substrate pre-treatment.[6] This presentation will highlight the development of a new method to hydrolyse various chitinous materials into GlcNAc using an inexpensive commercial chitinase in the absence of bulk solvent.

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Felix Saraci
Concordia University

Rare-earth Metal–Organic Frameworks (RE-MOFs) as fluorescent-based chemical sensors for applications in the detection of antibiotic contaminants in water

Authors: Felix Saraci, Dr. Ashlee J. Howarth*

Organics, inorganics, and antibiotics are among some of the most common pollutants found in water; leading to a current rise in the development of numerous techniques used to detect and remove them. Rapid and selective approaches for identifying contaminants in water are vital in overall treatment and monitoring; however, current methods of detection are either too strenuous, time-consuming or expensive.[1] A chemical sensor can continuously monitor the existence of a chemical species and is a durable and effective method of choice for the detection of analytes.[2] Fluorescence-based chemical sensors (FCS) are a class of strong candidates for chemical sensing due to their fast response time, high sensitivity, and easy-to-use handling. Metal–organic frameworks (MOFs) are a class of unique crystalline porous materials that are composed of metal nodes or clusters, and organic linkers that have been studied extensively due to their high functionality in various applications, which include catalysis, gas-storage, and chemical sensing.[3] MOFs can provide a tunable and robust platform as chemical sensors, mainly as fluorescent-based MOFs used in the detection of pollutants in water. Herein we present a novel class of rare-earth (RE) based MOFs that are comprised of yttrium, europium, terbium, or ytterbium (Y^{3+}, Eu^{3+}, Tb^{3+}, or Yb^{3+}) and commercially available linkers. These RE(III)-based MOFs are a new class of rare-earth MOFs, represented as CU-22 and CU-23 that demonstrate the potential for the detection of contaminants in water through fluorescent properties.

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Filip Topić
McGill University

Efficient recognition of steroids by planar aromatic molecules: Exploring the building block landscape and potential applications of a novel biomolecular recognition motif

Authors: Filip Topić, Tomislav Friščić

Traditionally, functional groups attached to the backbone of steroid molecules were seen as the key factors in their molecular recognition and, consequently, its physiological function. However, a systematic study of the cocrystals of steroids with electron-rich, planar aromatic molecules (arenes) by our group has recently revealed the α···π interaction:[1] a previously undescribed interaction mode of steroids involving the α-face of a steroid and the π-electron system of aromatic molecules. Progesterone was found to reliably engage in α···π interaction with various arenes, whereas other steroids studied so far suggest a strong dependence of this interaction on the fine structural details of the steroid backbone. This mimics the steroid behavior in the biological systems, where small structural differences give rise to significantly different biological functions. We set out to pursue the cocrystallization of progesterone with a variety of polyaromatic hydrocarbons and heterocycles using the mechanochemical solid-state screening methods developed in our group.[2] Furthermore, we sought to expand the set of steroid cocrystal formers towards biologically and pharmaceutically relevant adrenosterone (a weak androgen), cholest-4-en-3-one (metabolite of cholesterol), exemestane (anticancer drug) and levonorgestrel (used in birth control), all of which exhibit a degree of structural similarity with progesterone. Finally, we investigated the possibility of combining the α···π interaction with known interactions such as hydrogen and halogen bonding to engineer increasingly complex molecular solids.

This presentation will outline our initial findings, which confirm the reliability of the α···π interactions and establish its applicability to steroid molecules beyond progesterone.

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Francisco Yarur
Concordia University

Visible-Light Sensitization of Inorganic Semiconducting Nanostructures for Photoelectrochemical Energy Conversion

Authors: Francisco Yarur Villanueva, Marek B. Majewski*

The detrimental effects of the use of fossil fuels have brought about the need to develop sustainable and renewable energy technologies to supply the energetic demands of a carbon-neutral society. Converting solar energy into chemical fuels (i.e. artificial photosynthesis) and industrially relevant chemicals or organic compounds is an attractive alternative to address the global energy problem. Artificial photosynthetic systems require, amongst other things, a high stability under continuous light irradiation and the use of Earth-abundant elements to make these technologies economically feasible. The use of metal oxide nanomaterials as semiconductors has attracted significant attention within the past few decades due to their stability, low cost, high surface area, and ability to absorb light from different parts of the solar spectrum. However, the use of these materials for artificial photosynthesis is partially hindered by their limited absorption range in the solar spectrum and high rates of electron recombination within the material. In this work, we explore options to maximize the light harvesting properties of zinc oxide nanowires and how to minimize electron recombination while using different solar fuels co-catalysts.

Ghada Ayoub
McGill University

Mechanochemistry, accelerated aging, or both? Solid-state synthesis of edible MOFs

Authors: Ghada Ayoub, Gemma M. Garwell, Tomislav Friščić

Metal–organic framework materials have been intensively studied due to their outstanding potential[1] in many applications, ranging from catalysis, gas storage and separation, drug delivery, etc.[2] Nevertheless, to be implemented in biologically-targeted applications, the functional framework should be comprised solely of benign, safe starting materials, that are also biocompatible and, ideally, inexpensive.[3] The herein presented work demonstrates the synthesis of MOFs from naturally available building blocks such as gamma cyclodextrin (γ-CD), a symmetrical cyclic oligosaccharide derived from starch. Moreover, γ-CD is a feasible alternative to traditional MOF linkers, as it possesses a potentially bidentate metal-bonding motif through its primary and secondary faces that are able to coordinate to mono- and divalent metals to form γ-CD MOFs. The presented synthesis is significantly more environmentally-friendly from the conventional solution-based routes, as it is completely solvent-free, and proceeds with minimum input of energy.[3,4] This presentation will outline not only the first solvent-free synthesis[5,6] of “edible MOFs” from γ-CD units and suitable alkaline and alkaline earth metal cations, yielding highly crystalline and porous materials, but will also describe supramolecular frameworks that are isoreticular to the as-synthesized MOFs, but do not involve metal ions.

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Hudson Bicalho
Concordia University

Development of Eu- and Zr-MOFs for Environmental Applications

Authors: Hudson A. Bicalho, Ashlee J. Howarth*

The population growth along with the exponential rise in industrial development have been causing serious damage to our living environment. In particular, the presence of emerging contaminants (ECs) in groundwater, surface water or even in drinking water, is raising concerns about the harmful effects of these contaminants on human health and for the environment. Since many ECs are resistant to biodegradation, other approaches should be performed, such as adsorption or advanced oxidation processes (AOPs). In light of this, great efforts have been made to develop new materials with efficient adsorptive or catalytic properties for the removal of ECs from water.

Over the last 30 years, metal–organic frameworks (MOFs) have attracted significant attention due to their outstanding properties, which include a large internal surface area, extensive porosity, high degree of crystallinity and remarkable chemical, thermal and mechanical stability. These materials are formed by metal cations or metal clusters (node) connected by multiple organic ions or molecules (linkers) giving rise to infinite three-dimensional framework. Thereby, considering the variety of metal ions and organic linkers that can be used and also the possibility of varying some reaction parameters – including temperature, pH, modulator, etc. – to achieve specifics properties or topologies, the synthesis of MOFs has infinite possibilities. Because of their special characteristics, MOFs have shown a wide array of potential application, such as gas storage, ion-exchange, catalysis, chemical sensing and removal of toxic substances from water. In this work we develop new MOFs comprised of Eu(III) or Zr(IV) metal nodes. Along with the synthesis, materials characterization will also be presented, including XRD, BET, IR, SEM, TGA, ICP-OES and NMR spectroscopy. In addition, the potential applications of these MOFs as chemical sensors and adsorbents for pharmaceuticals, hormones and dyes from water will be discussed.

Jean-Louis Do
Concordia University, McGill University

Exploiting the Flexible Interactions of Salicylic Acid-Based Helicates in the Synthesis of New Metal–Organic Materials

Authors: Jean-Louis Do, Tomislav Friščić, and Louis A. Cuccia

Helicates are molecular materials consisting of metal- and/or organic-based components bridged through non-covalent interactions to form helical complexes. These materials have gained tremendous attention over the years due to their versatility and relevance in the field of supramolecular chemistry, contributing notably towards our understanding of self-assembly, molecular recognition, interactions with biologically relevant molecules, and catalysis.[1-3] Studies on such compounds, however, have largely focused on their ability to encapsulate other molecules within their helical cavity and their templated self-assembly, typically in a solvent medium. Supramolecular helicates have been poorly investigated as templates, components, and structure directing agents in the assembly of new, functional, and crystalline solid materials for pharmaceutical, materials, and catalytic applications.[4-5]

Herein, we propose the design and study of helicates based on ligands derived from salicylic acid, directed towards new functional solids. Salicylic acid, as a precursor to aspirin and used in cosmetics and pharmaceuticals, is an industrially relevant chemical produced on a ton scale annually whose chemistry has thus been well studied. The goal is to exploit the ease of synthesis and flexibility of salicylic acid and its derivatives as building blocks to prepare new supramolecular helicates whose structural designs may readily be adapted to the assembly of materials with potential applications in catalysis, drug delivery, light harvesting, and porosity.

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Jogirdas Vainauskas
McGill University

Engineering Azulene-based Dichroic Cocrystals Using Halogen Bonding

Authors: Jogirdas Vainauskas, Filip Topić, Oleksandr S. Bushuyev, Christoper J. Barrett* and Tomislav Friščić*

Halogen bonding (XB),[1] a highly directional interaction formed between an electron-deficient halogen atom as a donor and an electron-rich atom or a group as an acceptor, has proved to be a versatile tool for the assembly of cocrystals. Often forming with electronegative atoms such as oxygen or nitrogen, XBs also form with aromatic π-systems, such as in the previously described cocrystal of naphthalene and 1,4-diiodotetrafluorobenzene.[2] Through replacement of naphthalene by its constitutional isomer, intensely blue-colored azulene, we hypothesized that structurally analogous, di- or pleochroic materials could be formed.

Through screening by mechanochemical methods, a new class of molecular cocrystals is developed, based on using either azulene or a combination of azulene with an azobenzene-based chromophore, exhibiting dichroic and pleochroic behavior, respectively.

The herein presented results expand on our group's previous reports of using halogen bonds to generate dichroic crystalline materials[3-4] and represent a further advance in using XB-based crystal engineering to develop advanced optical materials.

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John Hadynski
Clarkson University

Design and Synthesis of Zwitterionic Metal–Organic Frameworks

Authors: Shefa Alomari, John Hadynski

Metal–organic frameworks (MOFs) have emerged as a new type of porous material. Their crystalline structures are composed of metal clusters connected by polytypic organic linkers. The characteristics of the metal and organic ligand blocks are important for controlling the resulting topologies, pore environments, and functionalities and hence affect the characteristics of the MOFs to capture specific guest molecules. As a new means to introduce charged-polarized porosity into MOFs we explore zwitterionic (ZW) ligands as MOF building blocks. These ligands are composed of both cationic and anionic functional groups resulting in an electrostatic field gradient on their molecular surfaces. Incorporating them into MOFs leads to polarization effects on guest molecules, resulting in enhanced adsorption enthalpies and multi-stimulus-responsive properties. N-substituted pyridines, namely pyridinium and their derivatives are among the most famous zwitterions; however, the design and synthesis of new pyridinium-based ligands are challenging. In our research, we explore the synthesis of new rigid zwitterionic ligands through multi-non-standard organic protocols. In this poster presentation, we will present on the crystal structures and physical properties of new ZW MOFs. We will show that these systematic investigations will pave the way to develop new functional materials with improved adsorption properties.

Joseph Marrett
McGill University

Modulation of hypergolic behavior in MOFs via changes in solid-state structure

Authors: Joseph M. Marrett, Hatem M. Titi, Mihails Arhangelskis, Robin D. Rogers, Tomislav Friščić

The development of new hypergolic fuels, materials which ignite spontaneously on contact with an oxidizer, is of considerable importance for development in the aerospace industry, as the traditional hydrazine-based hypergols are toxic, carcinogenic, and pose a significant threat to the environment. Recent work in our group[1] presents a family of porous and isostructural metal–organic frameworks based on divalent metal cations and imidazolate linkers functionalized with vinyl or ethynyl groups which act as triggers for inducing hypergolicity. This presentation will outline subsequent work to determine the effect of MOF structure on hypergolicity via the synthesis of dense, non-porous analogous to these porous MOFs by mechanochemical and other types of synthesis. The study of these higher-density MOFs will allow for the elucidation of additional parameters for tuning of hypergolic performance, porosity and density, allowing for greater control over energetic properties when designing these materials for aerospace applications.

[1] Titi et al. Sci. Adv., 2019.

Joseph Ricardo-Noordberg
Concordia University

An Inexpensive Photochemical Cell Towards the Photocatalytic Generation of High Value-Added Chemicals

Authors: Joseph Ricardo-Noordberg, Marek B. Majewski*

Zinc and copper oxides are well studied materials in the context of solar energy conversion due to their low toxicity and high abundance. The combination of ZnO, an n-type semiconductor, and Cu_2O, a p-type semiconductor, results in the formation of a p-n junction. The p-n junction allows the effective separation of charge carriers upon photoexcitation, resulting in reduced charge carrier recombination and higher cell efficiency in photovoltaic cells. This junction is formed first by the hydrothermal deposition of the n-type ZnO nanowire array onto a transparent, conductive, fluorine doped tin oxide (FTO) substrate. The p-type Cu_2O is then electrodeposited onto the nanowire array, creating a high surface area p-n junction. The high abundance and low toxicities of the materials used, along with the accessible synthetic methods lead to the potential for a high degree of scalability. Furthermore, the Cu_2O band gap of 2.17 eV results in the absorption of visible light at wavelengths ≤ 570 nm. With the help of surface bound catalysts, these semiconductor films can potentially be used for the photochemical generation of high value-added chemicals such as $S_2O_8^{2-}$, Cl_2, or H_2O_2.

Kayrel Edwards
McGill University

Preparing cellulose-based stimuli responsive hydrogen-bonded materials

Authors: Kayrel Edwards, Christopher Barrett

Many photo switchable materials have azobenzene incorporated covalently into their backbones because the reversible trans-cis isomerization of azobenzene makes it an effective photo switch. However, systems using non-covalent interactions, such as hydrogen bonding, have garnered much attention due to the relatively strong, selective and directional nature of the hydrogen bond, and added reversibility to such systems. It has already been shown that when azobenzene is hydrogen bonded to a polymer, the physical, optical and mechanical properties of the polymer can be changed with light. The majority of the polymers utilized in making these supramolecular hydrogen bonded azobenzene systems however have been synthetic polymers.

Instead of using synthetic polymers to develop these supramolecular complexes, bio-degradable and bio-sourced polymers can be used, which offer both environmental and bio-compatable advantages. One of the most abundant natural polymers in the world is cellulose, which can be acetylated to form triacetyl cellulose (TAC), and has been shown to function as a good polymer matrix for the dispersion of Disperse Red azo dyes. Not only can dyes be incorporated into the cellulose-based matrix via hydrogen bonding, but the incorporation of the dyes into the matrix can be controlled using a stimulus, such as light or humidity.

Therefore, we prepared hydrogen bonded self-assembled guest-host complexes by mixing a range of substituted azobenzenes with triacetyl cellulose. These materials displayed improved optical and mechanical properties when compared to the host polymers and were also capable of assembly and controlled disassembly. The materials were characterized using solid state NMR and FT-IR spectroscopy, and the photo-induced kinetics of the trans-cis isomerization was studied.

Louae Abdulla
University of Windsor

Polymorphism in Xylazine HCl: A Solid-State NMR and DFT Study

Authors: Louae M. Abdulla, Austin A. Peach, Sean T. Holmes, and Robert W. Schurko*

More than 80% of pharmaceuticals are manufactured and consumed as solid materials.[1] The physicochemical properties (e.g., bioavailability, shelf-life, solubility, etc.) of active pharmaceutical ingredients (APIs) differ between solid forms, such as polymorphs, pseudopolymorphs, and amorphous solid dispersions;[2] hence, there is great interest in the rational design and screening of new solid forms with desirable/enhanced properties. To produce such materials, a deep understanding of the molecular-level structure of solid APIs is required, which could be assisted by characterization techniques like X-ray diffraction (pXRD) and solid-state NMR (SSNMR) spectroscopy.

SSNMR often provides deep insight into molecular-level structure, dynamics, and reaction mechanisms involved in the formation of different solid phases. Notably, SSNMR is extremely useful for probing dosage forms, in which signals from the API are often obscured by those arising from the much more abundant excipient matrix. Perhaps more importantly, the emerging field of NMR crystallography, which combines SSNMR spectroscopy with density functional theory (DFT) calculations and pXRD, shows great promise for the structural prediction and refinement of solid forms of APIs.[3,4]

Over 50% of APIs produced in the solid state are formulated as HCl salts;[5] as such, our group has developed ^{35}Cl SSNMR protocols that can be used for the identification of HCl API.[6] Xylazine HCl, a commonly used sedative in the field of veterinary medicine, has four known forms, including one hydrate and three anhydrous polymorphs. ^{35}Cl SSNMR experiments not only provide us spectral fingerprints for each form, but also allow us to examine the relationships between molecular-level structure and bulk physicochemical properties, and to pursue structural prediction and refinement using NMR crystallographic techniques.

Herein, we present a study of one hydrate and three anhydrous forms of xylazine HCl that are produced by mechanochemistry, recrystallization, and/or dehydration. First, we discuss the various synthetic methods for producing the four pseudopolymorphs. Second, we describe the use of ^{35}Cl SSNMR experiments to distinguish unambiguously between its hydrated and anhydrous forms. Each polymorph has a distinct Cl– environment with a unique hydrogen bonding network, and therefore, a distinct set of ^{35}Cl electric field gradient (EFG) tensor parameters, which provides a unique spectral fingerprint for each polymorph. Lastly, experimentally measured parameters are compared against those calculated from pXRD structures that are refined using the DFT-D2* method, which accurately predicts the hydrogen atom positions.[7] This study will prove useful for future NMR crystallographic studies on a wide array of HCl APIs.

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Love Karan
Université du Québec à Trois-Rivières

Efficient amide based luminescent metal–organic hybrids for selective detection of mycotoxins in food samples: Synthesis of hybrids and detection of toxins using photoluminescence studies

Nowadays, the main focus of the scientific community is to develop efficient chemical sensors for the detection of low molecular weight biomolecules as some of them have shown harmful effects on human health and the environment as well.[1] Among these biomolecules the mycotoxins which are produced by filamentous fungi belonging to the phylum Ascomycota regularly infect various food commodities.[2] Moreover, these toxins are mutagenic, teratogenic, and carcinogenic posing significant adverse health effects on human beings and animals as well [3]. In literature various detection methods based on immunochemical (ELISA), analytical (HPLC, UV, fluorescence and MS detectors) and some other methods such as (MIP's), electronic nose are reported.[4] Though these methods are effective however, they share common downside of high cost, complex sample preparation, and skilled staff. Therefore, it is required to develop convenient and cost effective detection methods for global food safety.

Optical sensing of the target molecules using fluorescence studies is a powerful detection method which involves either shift or quenching of fluorescence signal due to sensor analyte interactions.[5] The imperative factor for effective detection of analyte molecule is the choice of sensor material.[6] Accordingly, luminescent metal–organic frameworks (LMOF's) can serve as good candidate for detection purpose owing to enhanced fluorescence intensity (quantum yield) compared to organic ligand molecular chromophores alone due to immobilization of the later into 3D rigid framework. The resulting MOF has improved fluorescence efficiency due to the inhibition of non-radiative relaxation pathways (due to vibrational and rotational motions) of the chromophores. [7] Reports are available in the literature on the use of LMOF's as chemical sensors [8] while less work has been done on the utilization of LMOF's for mycotoxin detection.[7] Currently, we are presenting novel mixed LMOF's by using flexible amide based ligands and rigid tri and tetra carboxylic acids with transition metals viz. Cu(II), Co(II), and Zn(II) in order to evaluate their sensing ability towards mycotoxins using fluorescence spectroscopy. The reason for selecting amide based ligand is that the C=ONH moiety participates in hydrogen bonding interactions which may facilitate the detection of analyte molecules.

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Maria Matlinska
University of Alberta

Exploring Hydrogen Boding in Solids: Atomic Level Insight with Solid-State NMR

Authors: Maria A. Matlinska, Victor V. Terskikh, Roderick E. Wasylishen

Hydrogen bonding plays a critical role in the structure of many types of materials and is the most important of all directional intermolecular interactions.[1] It determines properties of biological compounds, such as protein folding and stabilizing the DNA structure, as well as determining the specificity of ligand binding – a property of interest for medicinal chemists and the pharmaceutical industry. Nevertheless, characterizing hydrogen bonding in solid state poses significant challenges.

Maleates – salts and esters of maleic acid, are central metabolites of plants, holding important roles in their physiology.[2] Also many drugs are available as maleic acid salts and esters, such as antihistamine chlorpheniramine maleate or methylergonovine maleate used to control postpartum hemorrhage. Another group of compond, beta-diketones, provide the best known examples of keto-enol tautomerism and 1,3-diketones are of interest to synthetic organic chemists, due to their accessibility, stability, and often unique properties. [3,4]

We illustrate how the strength of H-bonding and position of hydrogen in organic systems, such as selected esters of maleic acid and enol tautomers of 1,3-diketones can be assessed by investigating the deuterium isotope effects. We illustrate the versatility of solid-state NMR as a tool to investigate hydrogen bonding in solids. Our research combines NMR spectroscopy, X-ray crystallography and computational techniques to characterize intramolecular hydrogen bonds in solids, by utilizing isotope effects on magnetic shielding.

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Mehdi Esmaeili
University of Guelph

Short peptides as building blocks for soft materials

Authors: Mehdi Esmaeili, Aaron J. Smith, Dmitriy V. Soldatov

Our research is focused on the design of soft materials based on peptides. Short peptide molecules are versatile building units whose self-assembly can be directed to a desired hydrogen bonded framework. Such design can be accomplished through the choice of substituents on the peptide backbone, addition of suitable template molecules, or modification of the crystallization conditions. Peptide molecules are an excellent choice for crystal engineering of soft materials due to a number of properties: a) their ability to form numerous hydrogen bonds; b) restricted rotational freedom around the peptide backbone leading to a limited number of molecular conformations; c) the diversity of molecules that can be created through the replacement of residues, variation of the chain length, or incorporation of functional groups into the residues. Also, hydrogen bonds connecting the peptide molecules in the crystals are charge assisted and therefore thermodynamically stronger. At the same time, the bonds are kinetically easy to reverse and therefore the whole process can be effectively controlled by changing the temperature, concentration, pH, etc. Further, it is possible to design peptides that exhibit poor packing by themselves, which facilitates the incorporation of guest molecules. To illustrate the structural flexibility of soft materials based on short peptides, examples from our recent work will be presented.

Midhun Mohan
Université du Québec à Trois-Rivières

Synthesis of Novel Pyridone-based Metal–Organic Framework

Authors: Midhun Mohan, Adam Duong*

Metal–Organic Frameworks (MOFs) are polymers consisting of metal ions or clusters coordinated to organic ligands to form one, two or three-dimensional structures. MOFs are interesting because they possess diverse features such as porosity, functionality and structure, which makes them potential candidates for various applications such as gas storage and separation, catalysis, drug delivery, photoluminescence, magnetism, sensors, and so forth. So far, MOFs are mainly made with carboxylate ligands. Although, these MOFs have remarkable properties, they are usually thermally or chemically unstable and often are unrealistic in the industrial point of view due to the cost and complicated synthesis methods. This motivates us to explore other alternatives ligating groups to create stable and versatile structures of MOFs. In this work, we have synthesized a series of pyridone-based novel ligands to create new MOFs. From the point of view of coordination chemistry, pyridone ligating group is more versatile than carboxylate group. However, pyridone ligand is rarely used to prepare MOFs. As a proof of concept, we report a novel pyridone-based MOF-671. Data reveals that MOF-671 is synthesized in high purity and is thermally stable. This study can enlighten in opening a new era for MOF community to construct novel pyridone-based MOFs with exceptional properties

Mihails Arhangelskis
McGill University

Ab initio structure prediction of metal–organic frameworks

Authors: Mihails Arhangelskis, James P. Darby, Athanassios D. Katsenis, Andrew J. Morris, Tomislav Friščić

Metal-organic frameworks (MOFs) are microporous materials with emerging applications[1] in gas sorption, separation, catalysis, sensors, light harvesting etc. The versatility of MOFs stems from their modular nature, where the vast number of potential organic linkers and metal nodes can be combined to yield all kinds of net topologies, ranging in void size and shape, surface polarity, access to open transition metal sites etc.

The structural diversity of MOFs makes the design process challenging, requiring extensive experimental screening to select the combination of nodes and ligands yielding a structure most suitable for a particular purpose. Computational methods can greatly simplify the design process by providing stability rankings and property estimates for putative structures, reducing the time and cost of experimental screening.

Significant effort has been made to assess the topological preferences of MOFs[2] and predict their properties[3,4] computationally. Our work includes the application of periodic density functional theory (DFT) calculations to rationalize the sequence of MOF topological interconversions occurring under mechanochemical conditions,[5] explore the topological space of framework structures based on the recently isolated pentazolate (pnz-) ligand,[6,7] as well as perform a computationally-guided synthesis of a zeolitic imidazolate framework (ZIF), based on a fluorinated imidazolate linker.[8] So far, however, all computational studies relied on some form of prior structural knowledge, most notably Cambridge structural database (CSD) as a source of putative structures, thus limiting the search space to a set of previously reported topologies. This is in stark contrast to the field of porous molecular crystals, which has immensely benefited from ab initio structure prediction, where crystal packing is predicted solely from the knowledge of the molecular structure.[9]

In this presentation we will report our most recent efforts in MOF structure prediction, with examples from several MOF classes, including hexafluorosilicate, azolate, and carboxylate frameworks. In all cases, experimental structures were used to confirm and evaluate theoretical expectations, providing an important step forward in theoretical understanding as well as modelling of MOFs.

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Mitchell Nascimento
University of Victoria

Ring-Opening Polymerization of Cyclic Phosphonates: Access to Inorganic Polymers with a P(V)–O Main Chain

Authors: Mitchell A. Nascimento, Marius I. Arz, Vincent T. Annibale, Nicole L. Kelly, John V. Hanna, Ian Manners*

The development of new polymers based on p-block elements is of continued interest due to the possibility to find materials with unique properties which may lead to new applications in polymer and material science.[1] In this respect, polymers consisting of a main chain of P–O bonds with modifiable organic side chains may exhibit interesting properties, but have only been briefly noted in the literature. Here we describe a new class of inorganic polymeric materials featuring a main chain of alternating P(V)–O bonds and aryl side groups, which were obtained with >70 repeat units by ring-opening polymerization of 6-membered cyclic phosphonate precursors. This monomer-polymer system was found to be dynamic in solution enabling selective depolymerization under dilute conditions, which can be tuned by varying the substituents. The polymers show high thermal stability to weight loss and can be easily fabricated into self-standing thin films.[2]

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Mohammad Sharif Askari
Concordia University

Sodium Chlorate and Mirror Symmetry Breaking – A Historic Perspective

Authors: Louis A. Cuccia, Mohammad S. Askari, Pedro Cintas, Cristobal Viedma

Optical activity in isotropic crystals was first observed in 1854 by Marbach in hemihedral crystals of sodium chlorate. Since this time, sodium chlorate has played a privileged role in the fascinating chemistry and physics of chiral crystals, especially with regard to chiral symmetry breaking. This poster will highlight the chirality of sodium chlorate and explore the essential role it has played in key discoveries related to mirror symmetry breaking.

Mohini Ramkaran
McGill University

McGill Chemistry Characterization (MC^2) Facility

Authors: Mohini Ramkaran, Petr Fiurasek

The McGill Chemistry Characterization (MC^2) facility is a multi-user facility that provides instrumentation and expertise on a wide variety of analytical and microscopy techniques. Our instrumentation currently includes mass spectrometry, single-crystal and powder diffraction, NMR and EPR spectroscopy, AFM (including MFM and STM), and TGA, DSC, FTIR, and UV-Vis. We serve both the experienced and novice investigators and our services include training for independent use, analytical services and full support from our experienced staff.

Our facilities are currently located across McGill's Department of Chemistry in the Otto Maass building and the Pulp and Paper Research Centre, but we are in the process of moving into a renovated joint facility in the Otto Maass basement. We serve over 200 researchers from academia, government labs, and industry each year.

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Our facilities are currently located across McGill's Department of Chemistry in the Otto Maass building and the Pulp and Paper Research Centre, but we are in the process of moving into a renovated joint facility in the Otto Maass basement. We serve over 200 researchers from academia, government labs, and industry each year.

Monu Joy
Clarkson University

Metal–Organic Frameworks as Platforms for the Nanostructuration of Single Molecule Magnets: New Insights from HRTEM

Authors: Juby Varghese, Monu Joy

Next-generation computer technologies require ultrahigh-density data storage devices and quantum computing based on isolated spin-carriers, so-called molecular spintronics. Single-molecule magnets (SMMs) show great potential for such applications due to their unique magnetic properties. Their magnetic bistability allows switching from total spin up to total spin down on a molecular level where each molecule serves as a magnetic bit of information. The quest for the design of new SMMs with improved properties is ongoing, however, coupling of the nanoscale units to the macroscopic world remains a major challenge. Practical applications of SMMs require their organization in 2D or 3D networks while being in a protected environment to enable read-and-write processes. Metal–organic frameworks (MOFs), due to their porous nature and tunability, are excellent candidates to overcome this challenge. This work is the first systematic investigation exploring MOFs as platforms for the controlled nanostructuration of molecular magnets in both bulk polycrystalline powder and thin film forms. Subsequent characterization of SMM@MOF composites using HRTEM provides previously inaccessible visual structural insights into these nanomagnetic composites bringing us one step closer to the development of spintronic devices combining functional properties of both SMMs and MOFs.

Nadia Stephaniuk
University of Windsor

Crystal Engineering of Thiazyl-based Radical-Radical Co-Crystals

Authors: Nadia T. Stephaniuk, Mitchell A. Nascimento, Dr. Jeremy M. Rawson

Thiazyl radicals have been extensively studied for their unique magnetic properties, and as a result have been employed in the design and fabrication of both magnetic molecular materials, as well as paramagnetic ligands in coordination chemistry. Here we report a class of radical-radical co-crystals which exploit the favorable structure-directing interactions of the E-E bond (E = S, Se) of dithiadiazolyl (DTDA) and diselenadiazolyl (DSDA) radicals with electronegative groups, such as the oxygen of a TEMPO radical, or the nitrogen of a methyl benzodithiazolyl radical to generate new radical-radical cocrystals. These have been characterized by EPR spectroscopy, powder X-Ray diffraction, and single crystal X-Ray diffraction.

Nour Dissem
Institut de Recherche sur l'Hydrogène, Université du Québec à Trois-Rivières

Synthesis and characterization of a new Cu(II) 3D coordination polymer from a mixed ligand synthetic approach

Authors: Nour Dissem, Adam Duong*

Coordinating polymers form an infinite number of crystalline materials in multidimensional metallo-organic networks whose interest continues to intensify with the endless possibility of modifying the structures at the molecular level and the properties of the resulting materials. These materials have many potential applications in various fields of science such as catalysis, magnetism, energy storage, separation and purification, CO_2 sequestration and so forth.

The combination of macrocyclic complexes of transition metals with aromatic polycarboxylates has proved to be a very particular field of research. Indeed, the carboxyl groups could induce plurivalent coordination modes with the macrocyclic complexes and could act as donors and / or acceptors of hydrogen bonds via inter and / or intramolecular manner for extended structures with distinctly aimed applications and properties. In this context, we chose to work with the copper polymer complexes using a tetradentate macrocyclic ligand (cyclam: 1,4,8,11-tetraazacyclotetradecane) and an aromatic ligand PMDA (pyromellitic dianhydride). The two different types of copper ions in the octahedral environment as well as the 1,4-COOH coordination mode of the aromatic ligand induces a three-dimensional network of crosslinked coordination polymer. The compound was characterized by single crystal X-ray diffraction (SCXRD) and powder (PXRD), infrared spectroscopy (IR), energy dispersive analysis (EDS) and thermal analysis (ATG-ATD). The magnetic properties of this material will also be studied.

Oliver Bleton, Ismael Elhasadi, and Amandeep Thind
Concordia University

Materials and Pharmaceutical Applications of Chiral Supramolecular Assemblies

Authors: Oliver Bleton, Ismael Elhasadi, Amandeep Thind, Jean-Louis Do, Tomislav Friščić, and Louis A. Cuccia

Supramolecular assemblies, i.e. complex yet discrete structures such as molecular polygons and polyhedra, consisting of discrete metal-based and/or organic species brought together by intermolecular forces hold great potential in various areas of chemistry (Figure 1). These materials have been used to trap and enable the study and isolation of reactive molecules,[1] effectively mimic the catalytic activity and selectivity of enzymes,[2] and interface with and target biological molecules such as guanine quadruplexes[3] among other applications. Supramolecular assemblies exhibiting chirality as a consequence of being made from inherently chiral components or from crystallization of achiral components into chiral crystalline forms are particularly interesting due to their potential for enhanced sensing, optical, electronic, and catalytic properties.[4,5]

Such materials are not without drawbacks, however, particularly in their synthesis, isolation, and purification. Herein, we highlight the design and study of chiral supramolecular assemblies. We will highlight previous work that has been carried out on select systems, the motivation behind their development, and their contributions towards the field of supramolecular chemistry. We will discuss the utility and applications of such materials, challenges encountered, and how we may apply these concepts towards the rational design of new chiral supramolecular assemblies.

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Olivier Schott
Université de Montréal

Supramolecular photochemistry towards solar hydrogen generation: Ir and Ru photosensitizers with Cobaltoximes

Authors: Olivier Schott, Garry S. Hanan

Nature has been using sunlight as its main energy source to oxidize water and fix CO_2 to produce carbohydrates for over a billion years. Molecular artificial photosynthesis aims to mimic nature by extracting electrons from water and reducing protons or others organic compounds (CO_2...) in order to store solar energy in chemical bonds.[1] Since the combustion product of hydrogen is water, this chemical conversion acts as a promising solution for renewable energy. Tuning the properties of molecular photocatalytic center by the design of metal-ligand interaction shows infinite possibilities of creation.[2] Here, we highlight the high photocatalytic activity of supramolecular Ru-Co and Ir-Co system for hydrogen generation. The electronic distribution of heteroleptic and homoleptic bidendante amide Ru complex[3] is investigated trough new derivatives for red-shift absorption, photoredox-reversibility and efficiency. Unstudied macrocyclic cobaltoxime derivatives prove high robustness for hydrogen evolution. Under various wavelengths of irradiation, the behavior of photo-catalytic activity is discussed to develop mechanistic advances.

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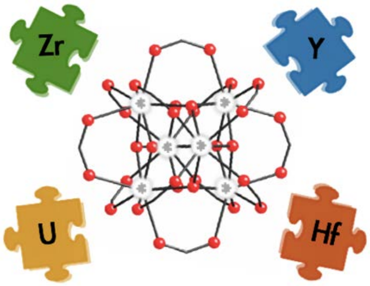
Paola Marino and Zvart Ajoyan
Concordia University

Functional Hexanuclear Cluster-Based Metal–Organic Frameworks: From Materials Design to Application

Authors: Paola Marino, Zvart Ajoyan, Ashlee J. Howarth*

Metal–organic frameworks (MOFs) are an innovative class of hybrid porous materials that are comprised of metal nodes and organic linkers. MOFs can be designed and synthesized to have specific topologies and to present important structural features that may be of use for a wide array of applications. By varying these structural characteristics, applications can be specifically targeted, and versatile properties such as tunable pores, surface areas and stability, can be predicted, understood, and improved. Hexanuclear cluster-based MOFs such as those comprised of Zr_6, Hf_6, Y_6 and U_6 nodes (among others) are an important class of highly robust MOFs with topologies dictated, in part, by the octahedral node structure.[1]

The use of reticular chemistry, pertaining to crystal engineering and topology-guided design, has paved the way for the controllable design of hexanuclear MOF structures to be used for target applications, including but not limited to gas storage and release, wastewater remediation, and catalysis.[2,3] Herein, this poster presentation will highlight the design rules that have been used for synthesizing MOFs with the hexanuclear building block, post-synthetic strategies for tuning these MOFs and potential applications for the MOFs-by-design.



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Patrick Julien
McGill University

Monitoring Mechanochemical synthesis of cocrystal fertilizers reveals water mediated feedback mechanism

Authors: Patrick A. Julien, Jonas Baltrusaitis, Tomislav Friščić

Co-crystal forms of important agrochemicals such as urea are being synthesized mechanochemically to improve properties such as nitrogen uptake and minimize eutrophication.[1] Real-time reaction monitoring via both Raman spectroscopy[2] and synchrotron X-ray powder diffraction[3] are applied for the first time for agriculturally relevant cocrystal materials and reveals considerable differences in reaction kinetics between carbonate and hydroxide precursors for the formation of calcium urea phosphate. We present direct evidence of a system where water mediates the rate of transformation and underpins the positive feedback kinetics typical of mechanochemical reactions.

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Pedro Donnarumma
Concordia University

Rare-earth based fcu Metal–Organic Frameworks for aqueous contaminants degradation

Authors: Pedro Donnarumma, Ashlee J. Howarth*

Metal–organic frameworks (MOFs) are a family of structurally diverse materials made up of both inorganic and organic components. The permanent existence of pores in their structures and their low density makes their potential for applications wide ranging - from the field of gas storage to light harvesting and energy conversion.

The formation of a hexanuclear rare-earth (RE) based cluster opens up the door for a diverse class of robust functional MOFs. It is possible to use these clusters as metal nodes and, through the use of organic linkers that are linear and ditopic, obtain a framework with **fcu** topology.

Antibiotics are amongst the most successful treatments for improving human, animal and plant health. Nonetheless, the ubiquitous use of antibiotics has led to their release in natural ecosystems. Although their effects on natural ecosystems can be many, one of the most detrimental is the development of mutagenic, multi-antibiotic resistant bacterial strains that can produce untreatable infections that affect mainly aquatic life.

This presentation will discuss the synthesis and full characterization of rare earth MOFs with **fcu** topology and their potential for use in the catalytic breakdown of antibiotics in water.

Petr Fiurasek
Québec Centre for Advanced Materials

Centre Québécois sur les Matériaux Fonctionnels (CQMF) - Quebec Centre for Advanced Materials (QCAM)

Authors: Petr Fiurasek, Michel Lafleur, Theo van de Ven, Matteo Duca

Le Centre Québécois sur les Matériaux Fonctionnels (CQMF) est un regroupement stratégique du Fonds de recherche Nature et technologies. Avec 97 chercheurs et plus de 600 étudiants (incluant des stagiaires postdoctoraux), c'est un des plus grands centres en science et ingénierie des matériaux au Canada. Dans la vaste thématique des matériaux fonctionnels, le CQMF concentre ses activités autour de trois axes de recherche fondamentale, la chimie des polymères, l'auto-assemblage moléculaire et les nanosciences, permettant ainsi de développer des matériaux, des dispositifs et des technologies répondant à des besoins spécifiques de notre société, représentés par ses axes de recherche appliqués: les applications biomédicales, énergétiques et environnementales.

The Quebec Center for Advanced Materials (QCAM) is a strategic research cluster funded by the Fonds de recherche Nature et technologies. With 97 researchers and more than 600 students (including postdoctoral fellows), it is one of the largest materials science and engineering centers in Canada. Activities are focused around three fundamental research themes, polymer chemistry, molecular self-assembly, and nanoscience, to develop materials, devices, and technologies for the critical societal needs represented by our applied research axes: advanced materials for biomedical applications, energy, and environment and sustainable development.

Robin Stein
McGill University

McGill Chemistry Characterization (MC^2) Facility

Authors: Petr Fiurasek, Mohini Ramkaran, Nadim Saadeh, Robin Stein, Hatem Titi, Alexander Wahba

The McGill Chemistry Characterization (MC^2) facility is a multi-user facility that provides instrumentation and expertise on a wide variety of analytical and microscopy techniques. Our instrumentation currently includes mass spectrometry, single-crystal and powder diffraction, NMR and EPR spectroscopy, AFM (including MFM and STM), and TGA, DSC, FTIR, and UV-Vis. We serve both the experienced and novice investigators and our services include training for independent use, analytical services and full support from our experienced staff.

Our facilities are currently located across McGill's Department of Chemistry in the Otto Maass building and the Pulp and Paper Research Centre, but we are in the process of moving into a renovated joint facility in the Otto Maass basement. We serve over 200 researchers from academia, government labs, and industry each year.

Sandra Kaabel
McGill University

Anion-templated dynamic covalent self-assembly of hemicucurbit[n]uril macrocycles in the solid state

Authors: Sandra Kaabel, Robin S. Stein, Maria Fomitšenko, Ivar Järving, Riina Aav, Tomislav Friščić

Chiral cyclohexanohemicucurbiturils (cycHC[n]) are barrel-shaped macrocyclic receptors, potentially useful for anion sensing, transmembrane anion transport and asymmetric catalysis, due to the selective and strong encapsulation of anions and electron-rich guests.[1] The synthesis of 6- and 8-membered cycHC[n] proceeds in strongly acidic solutions, through dynamic covalent chemistry, where the target macrocyclic product is dictated by the choice of the anionic template.[2,3] Recently, we found that selective macrocyclization to cycHC[n] can also be achieved using solvent-free approaches, by combining ball milling and aging.[4] The novel approach for the synthesis of cycHC[n] proceeds selectively and quantitatively from the cyclohex-1,2-diylurea monomer and paraformaldehyde in a template-directed process, providing a first clear example of supramolecular templating in mechanochemically-activated dynamic covalent solid-state reactions. Liquid-assisted grinding (LAG) of the reactants with a catalytic amount of acid produces a solid mixture of oligomers which spontaneously self-organize into a single macrocyclic product, directed by the choice of the LAG acid. Besides providing a cleaner and safer route for the synthesis of the macrocycles, by removing the bulk of used acid and solvents, these processes contribute to the understanding of solid-to-solid transformations that rely on thermodynamic self-assembly.

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Sanil Rajak
Université du Québec à Trois-Rivières

Catalyst Design For Photochemical Hydrogen Evolution Reaction

Authors: Sanil Rajak, Olivier Schott, Garry Hanan, Adam Duong*

With the depletion of fossil fuels and the phenomenon of global warming, the necessities for the development of clean and sustainable energy sources are imperative. H_2 is a clean, environmentally benign and sustainable energy carrier as water is the only side product after combustion. Additionally, as fuel hydrogen possesses greatest energy output relative to the mass. However, molecular hydrogen is very rare in the Earth's atmosphere c.a. 1 ppm by volume. Therefore, it needs to be produced from suitable sources. Sunlight-triggered hydrogen evolution reaction (HER) has proven to be an interesting solution to harvest the abundant and inexhaustible power of solar energy in the form of chemical bonds. A typical hydrogen evolution reaction is based on visible light induced sensitization of photosensitizers from which the electrons are transferred to the photo catalytic centre to produce hydrogen with the help of a sacrificial electron donor (SED). Ruthenium and cobalt complexes are one of the most studied and reported complexes as photosensitizers and photo catalysts respectively. However, the design and development of highly efficient and non-expensive molecular catalysts and the modification of the catalysts by effective and low-cost ligand design remains the largest focus of research. Here we have developed the synthesis of several novel molecular catalysts based on transition metal complexes for visible-light driven hydrogen evolution reaction (HER) by employing the strategy of metallotectons which are comparatively easy and less expensive to synthesize.

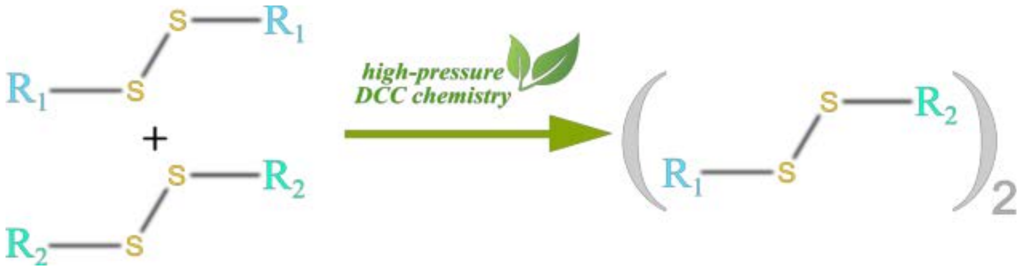
Szymon Sobczak
Adam Mickiewicz University

Mass spectrometry as a tool for controlling products of high-pressure disulphide metathesis reaction

Mass spectrometry is an essential analytical technique and it has gained great popularity due to such features as unequalled sensitivity, speed and variety of other applications. This fast method is commonly used in drug discovery, in pollution and food control or in forensic science.[1]

In our experiments, we have used mass spectrometry to identify the products of high-pressure metathesis reactions. This reaction is the first example of a reaction in which the high-pressure is used instead of a catalytic or reducing agent.[2] At ambient conditions, this reaction can be conducted with high efficiency either by ball mill grinding or by liquid assisted grinding, however in both this processes the additional catalysts is required.[3] In our studies, we have investigated metathesis reactions between p-tolyl disulfide, 4-chlorophenyl disulfide, 2-aminophenyl disulfide and 2-nitrophenyl disulfide. All pressure-induced disulfide metathesis reactions were conducted in the diamond-anvil cell.

To confirm that the reaction occurred and expected products were obtained, mass spectrometry was used. By using this quick method, we can immediately improve the yield of reaction and what is more important, their selectivity by changing concentration, pressure or used solvent. What is more, choosing the right conditions is extremely important for obtaining high-quality single crystals, which can be further characterized by single-crystal X-ray diffraction measurements.



Acknowledgments: This work was supported by funding from the Polish National Science Centre (Preludium No. 2017/27/N/ST5/00693)

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Tomislav Friščić
McGill University

Remembering Joel Bernstein: The archetype of cocrystal-mediated solvent-free synthesis

Authors: Angela Novakovic, Hatem M. Titi, Lois Overvoorde, Ian R. Baxendale, Laszlo Fabian, Robin S. Stein, Tomislav Friščić

The archetypal example[1] of a solvent-free synthesis through thermochemical formation of covalent bonds in a cocrystal obtained by mechanochemical grinding[2] was re-investigated with the aid of variable temperature X-ray powder diffraction and structure determination from powder diffraction data. Our studies reveal that the reactivity in this historically important system, discovered two decades ago by M. C. Etter, is the result of an interplay of high-temperature polymorphism and solid-state topochemistry.

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Victor Quezada
Concordia University

A New Metal–Organic Framework synthesized from Yttrium and a Tetratopic Linker

Authors: Victor Quezada, Hatem Titi, Ashlee J. Howarth*

Metal**–**Organic Frameworks (MOFs) are porous crystalline materials that have been intensively studied in the last two decades due to their applications in gas adsorption, catalysis, water remediation, among others.[2] The properties of MOFs are driven by the organic linkers (L) and metal (M), what are they made of, and their spatial arrangement along the structure.[2] In this work, we expose the solvothermal synthesis of a new MOF, based on a well-known linker and yttrium as the metal node, obtaining a structure that has never being reported before, which will be a staring point to study the properties of these kind of metal complexes.

Single-crystal X-ray diffraction (SXRD) resolved until now, shows that the MOF has triangular 1D channels along the “c” axis. Additionally, several bulk syntheses have been carried on, and analyzed by Powder X-ray Diffraction (PXRD), demonstrating the reproducibility of the procedure. In this presentation, the MOF structure will be exposed, and full characterization of this new material presented (FT-IR, ^{1}H-NMR spectroscopy, TGA, N_2 adsorption). The stability of the MOF in water, acidic, and basic solutions will also be discussed, as well the potential applications of this new material.

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Zachary Schroeder
Wilfrid Laurier University

Synthesis of Polycyclic Aromatic Hydrocarbons via Yamamoto Cyclization

Authors: Zachary W. Schroeder, Lana Hiscock, Kenneth E. Maly*

Polycyclic aromatic hydrocarbons are a sought-after class of molecules for potential organic electronic applications.[1] Triphenylenes and trinaphthylenes in particular are privileged scaffolds due to their ability to self-assemble into hexagonal columnar liquid crystalline phases which have promising charge transport properties.[2] The Yamamoto cyclotrimerization reaction has proven useful for the preparation of these trimeric systems.[3] This reaction removes the need for the preparation of elaborately functionalized starting materials through direct trimerization of o-dibromoarenes.[4] Since these substrates may be accessed in very few, often high yielding steps, this reaction may effectively streamline the production of otherwise difficult to access trimers.[5] Herein, we explore the scope of the Yamamoto reaction for the preparation of a variety of triphenylenes and related polycyclic arenes. In particular, we aim to prepare electron deficient, sterically encumbered, and N-heteroacene based trimers.[5,6,7] Carefully selected starting substrates allow for the production of materials which possess interesting liquid crystalline, optoelectronic, and photophysical properties.[5,6,7]

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Zahir Razzaz
Laval University

Production and characterization of hollow fiber extruded foam membranes for gas separation

Polymer foams are an interesting class of materials with unique structures and properties for numerous applications. In this work, hollow fiber porous nanocomposite membranes were successfully prepared by the incorporation of a porous nanoparticle (zeolite 5A) into a blend of linear low-density polyethylene (LLDPE)/low-density polyethylene (LDPE) combined with azodicarbonamide as a chemical blowing agent (CBA). The results show that hollow fiber foamed membranes having a higher cell density can increase gas permeability, indicating a new realm of application for polymer foams. The results show that the developed cellular structure has a high potential for the continuous and cost-effective production of hollow fiber membranes for different gas separation, especially for hydrogen recovery.

Zujhar Singh
Concordia University

Synthesis and integration of donor-chromophore-acceptor (D-C-A) based Cu(I) triads onto semiconductor surfaces to drive single electron transfer (SET) processes

Authors: Zujhar Singh, Marek B. Majewski*

In recent years, photoredox catalysis has become an important tools to drive organic transformations or fuel forming processes (i.e. artificial photosynthesis). Regardless of substrate, photoredox catalysis begins with single electron transfer from a molecular assembly/chromophore/photosensitizer which upon photoexcitation produces a long lived charge separated state (CSS). Ruthenium and other 3rd row transition metals (Os, Re, Ir) have high CSS efficiencies, but these metals are toxic and less abundant whereas Cu(I) complexes are abundant, and show similar photophysical properties to Ru(II) complexes. Furthermore, the metal to ligand charge transfer (MLCT) state of Cu(I) can act as a strong reductant and can further be used to transfer a single electron to a target substrate. We are working on developing Cu(I) based D-C-A triads with specially tailored ligands having different electron donating and accepting moieties. These triads, upon visible light irradiation may give rise to MLCT states in high quantum yield which can further undergo reductive quenching to form charge separated states. We anticipate that this CSS can act as a single electron transfer cascade and can be used to transfer a single electron which can then be used by a proton reduction catalyst to generate hydrogen, drive organic transformations involving radical intermediates and simply as an exciton in solar cells. Furthermore, the D-C-A triad can be coupled to semiconductor surfaces to generate a dye sensitized photo electrochemical cell (DS-PEC) using a bottom up approach.

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Pedro Donnarumma	Concordia University
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