ChemCon 2019
Program

Acadia University
May 24-26, 2019
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Campus Map

Chase Court (Residence Accommodations)

KCIC (Registration and Presentations)

Wheelock (Meal Hall)

The Axe Lounge (Night Events)

Fountain Commons (Poster Presentations)
Map of Wolfville – Food and Drink
## Food and Drink—Wolfville

<table>
<thead>
<tr>
<th>$</th>
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</thead>
<tbody>
<tr>
<td>Chart’s Café</td>
<td>The Axe Lounge</td>
</tr>
<tr>
<td>16 Elm Ave.</td>
<td>30 Highland Ave.</td>
</tr>
<tr>
<td>Just Us!</td>
<td>The Church Brewing Co.</td>
</tr>
<tr>
<td>450 Main St.</td>
<td>329 Main St.</td>
</tr>
<tr>
<td>The Naked Crepe</td>
<td>Joe’s Food Emporium</td>
</tr>
<tr>
<td>406 Main St.</td>
<td>434 Main St.</td>
</tr>
<tr>
<td>Picasso’s Pizza</td>
<td>Li’s Wok and Grill</td>
</tr>
<tr>
<td>393 Main St.</td>
<td>112 Front St.</td>
</tr>
<tr>
<td>The Pita House</td>
<td>The Library Pub</td>
</tr>
<tr>
<td>389 Main St.</td>
<td>472 Main St.</td>
</tr>
<tr>
<td>Pronto Pizza</td>
<td>Paddy’s Pub</td>
</tr>
<tr>
<td>467 Main St.</td>
<td>460 Main St.</td>
</tr>
<tr>
<td>The Rolled Oat</td>
<td>La Torta Woodfired Pizza</td>
</tr>
<tr>
<td>402 Main St.</td>
<td>117 Front St.</td>
</tr>
<tr>
<td>T.A.N</td>
<td>Troy</td>
</tr>
<tr>
<td>378 Main St.</td>
<td>12 Elm Ave.</td>
</tr>
<tr>
<td>Tim Horton’s</td>
<td></td>
</tr>
<tr>
<td>370 Main St.</td>
<td></td>
</tr>
<tr>
<td>The Real Scoop—Ice Cream</td>
<td></td>
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<tr>
<td>10 Gaspereau Ave.</td>
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</tbody>
</table>
General Information

PIZZA AND TRIVIA
Free pizza and trivia will follow the first guest speaker, Dr. Peter W. Mullen, at the Axe. All are welcome to attend. There will be prizes!

PRESENTATIONS AND GRAD FAIR
Oral presentations will take place in the main auditorium of the K.C. Irving Environmental Science Centre (KCIC). Each will be limited to 10 minutes with a 5-minute question/discussion period. Presenters will be notified when 8 minutes have elapsed.

Poster presentations will be given at a designated space in Fountain Commons on May 25th, from 1:00 pm to 2:50 pm. The Grad Fair will take place in conjunction with the poster presentations.

WINE TOUR
There will be a free wine tour of Lightfoot and Wolfville Vineyards Saturday, May 25th. A bus will depart from the front of the KCIC at 7:15 pm taking those who are interest. We expect to return at the KCIC for approximately 9:00 pm.

BANQUET
The banquet will take place on Sunday Evening with a cost of $35.00 a person. The attire is formal.

BIDS FOR CHEMCON 2021
Bids for ChemCon 2021 will be made during the banquet on Sunday. Screens to display a presentation will be provided.
Message from the Conference Chair

Dear Attendees,

On behalf of myself and the organizing committee, it is my pleasure to welcome you all to the 44th Annual Science Atlantic Chemistry Conference (ChemCon). Our department is honoured to host this gathering of the best and brightest of Atlantic Canada here in Wolfville—the heart of the beautiful Annapolis Valley.

ChemCon is a vital component of the chemistry community in Atlantic Canada: it inspires students, facilitates the flow of knowledge between our many institutions, and forges new connections between students and faculty alike. This is achieved through a fun and information-filled weekend of student oral and poster presentations. In addition to student presentations, we are excited to have Dr. Peter W. Mullen and Dr. Belinda Kemp share with us some of the many applications of chemistry to our daily lives, reminding us that chemistry doesn’t only exist in the lab.

I would like to thank all of the sponsors and volunteers that helped make this conference a reality. Planning such an event takes a tremendous amount of work, which could not have been accomplished without a strong team. A special thanks to Dr. Bobby Ellis, our faculty advisor, for his guidance and help with the many intricacies of planning this conference.

To all attendees of ChemCon 2019, I encourage you to make the most out of this weekend: absorb the talks, attend the social events, talk to new people! I know I still remember every minute of the ChemCon I attended and look back on it fondly. I hope that you all make similarly fond memories and enjoy this special event. We’ve done our best to ensure this conference is as fulfilling as ever. Please feel free to contact myself, or anyone on the committee, with any questions you have.

Sincerely,

Alex Hebert
Chair, ChemCon 2019
Message from the Department Head

Dear Chemists,

Listening to a recent radio program, I have learnt that it could be an inherited predisposition to be liberally or conservatively oriented. That it is our brain that decides whether the same information makes perfect sense to some, while being complete nonsense for others. I recalled my Biology friends who insisted that everything is in our genes, ultimately in the way our DNA is put together...

This made me wonder, what if being a Chemist is also a part of our nature? What if it also requires a certain predisposition, a combination of DNA, to truly love Chemistry? To love it both as a science and an art, while for others it might be just a curse word...

As acting Head, I am pleased to welcome you to Acadia University and Chemistry Department to attend this inspiring information exchange. Let us learn from each other and promote respect to our favourite art and science. Have a great time!

Vlad Zamlynny, Ph.D.
Associate Professor and acting Head of Chemistry.
Organizing Committee

**Chair**
Alex Hebert

**Faculty Advisor**
Dr. Bobby Ellis

**Financial Coordinator**
Anna Crouch

**Fundraising Coordinator**
Alyson MacKay

**Volunteers**
Zainab Bello
Safyha Bryan
Kaela Fraser
Daniel Gawalewicz
Nick Harvey
Victoria Hopper
Alexis Mackey
Jocelyn Leon
James Mastin
Jenna McNutt
Joe Nazak
Emma Sutherland
Sarah Visser
Daniel Whalen
## Presenting Delegates

### Acadia University
- Alex Hebert
- Kaela Fraser
- Jun Luo
- Jenna McNutt
- Joseph Weatherby
- Erin Welsh
- Scott Young
- Tianjin Zhang

### CBU
- Sarah Boudreau
- Kuljit Kaur
- Rahul Pongasseresril

### Dalhousie University
- Michael Beh
- Clarke Brown
- Ziyi Chen
- Samantha Corkum
- Bry Crabbe
- David Do
- Dylan Hale
- Helia Hollenhorst
- Blake Huchenski
- Toren Hynes
- Alysson Jones
- Marcus Kindervater
- Sarah Martell
- Harrison Max
- David Morris
- Katherine Parsons
- Margan Payne
- Karin Reznikov
- Sydney Shepard
- Jeffrey Simmons
- Jamie Stark
- Emily Traver
- Andrew Walsh

### Memorial University
- Shayan Azher
- Sarah Clarke
- Evan Connors
- Dakshita Jagota
- Kirkland Lockyer
- Soraya Moore
- Lindsey Parsons
- Christopher Qiu
- Ryan Warren
- Craig Weir

### Mt. Allison University
- Annabelle Kilham

### Saint Mary’s University
- Kaitlyn Blatt-Janmaat
- Kennedi Brittain
- Jacob Campbell
- Julie Anne Dayrit
- Abdurrahman Elajmi
- Tanner George
- Jacob Hoare
- Ariana Joseph
- Jennifer Kolwich
- Prashansa Kooshna
- Matthew Laprade
- Brandon Logan
- Kaleigh McLeod
- Bailey Mosher

### StFX University
- Elvin Girineza
- Nikita Kenney
- Shannon MacLennan
- Tiffany MacLennan
- Dreenan Shea

### UNB - Fredericton
- Jordan Conrad
- Michel Deschenes
- Chun Keat Khor
- Ben Nadeau
- Jordyn Weddell

### UPEI
- Lauren Grant
- Anayet Kabir
- Tara Misener
- Liam Payne
- Holly Studzinski
- Chad Turner
- Timara Uhlig
Guest Speakers

Peter W. Mullen, Ph.D., FCSFS
Kemic Bioresearch

Peter W. Mullen received his first degrees (B.Sc. and B.Ed) from Acadia University. After completion of an M.Sc. in Forensic Science (Strathclyde), a Ph.D. in Pharmacology (Manchester) and postdoctoral research at the University of Edinburgh, he held a tenured faculty appointment at the University of Manchester Medical School. On behalf of Kemic Bioresearch, a research and consulting firm he established upon his return to Canada, he has presented courses in pharmacokinetics, toxicology and related disciplines at various venues internationally (Canada, USA, UK, Brazil). He has also taught courses at Acadia and Dalhousie Universities. Dr. Mullen has served as an expert witness re. forensic toxicological matters in the Provincial and Supreme Courts of Nova Scotia and Prince Edward Island, the Provincial Court of New Brunswick, the Supreme Court of Newfoundland and in Canadian military Courts-Martial. He has organized scientific conferences including a NATO Advanced Study Institute and the 1998 Annual Meeting of the Canadian Society of Forensic Science. Dr. Mullen is a fellow of the Canadian Society of Forensic Science and a member of many other scientific organizations. A former board member of the Nova Scotia Health Research Foundation and a former editor of the International Journal of Immunopharmacology, he currently serves on the editorial board of the International Journal of Clinical Pharmacology and Therapeutics.
Dr. Belinda Kemp, Ph.D.
Adjunct Professor, Brock University

Belinda Kemp gained her PhD at Lincoln University, New Zealand after studying Pinot noir tannin, flavour and sensory characteristics of wine. She is Senior Staff Scientist in Oenology at the Cool Climate Oenology and viticulture Institute (CCOVI) at Brock University and Adjunct Professor in the Faculty of Biological Science. As well as a scientist, Kemp gained previous practical still and sparkling winemaking experience in commercial wineries in New Zealand and the UK. Her main research areas are wine flavour and aroma. Her research since joining CCOVI has included sparkling wine research projects investigating the effect of sugar and dosage solutions on Niagara sparkling wine flavour and influences of sparkling wine clones and soil type on flavour. She is currently investigating cool climate red wine tannin management, and sparkling wines flavours during bottle aging. She currently organises FIZZ Club for Ontario sparkling winemakers to disseminate research results and serves on the VQA-O Wine Standards Development Committee and the VQA-O sparkling wine regulations committee.
Conference Sponsors

Gold
Acadia Chemistry Club
Acadia University Department of Chemistry
BioVectra Inc.
CIC Chemical Education Division
CIC Maritime Local Section

Silver
Acadia University Faculty of Pure and Applied Science
CIC Materials Chemistry Division
Paraza Pharma

Bronze
Acadia University
CIC Analytical Chemistry Division
CIC Newfoundland and Labrador Local Section
Federation of Canada’s Professional Chemists
Nova Scotia Chemists’ Society
Awards

- CIC Award for the Best Undergraduate Oral Presentation in Analytical Chemistry
- CIC Award for the Best Undergraduate Poster Presentation in Analytical Chemistry
- CIC Award for the Best Undergraduate Oral Presentation in Biological or Medicinal Chemistry
- CIC Award for the Best Undergraduate Poster Presentation in Biological or Medicinal Chemistry
- CIC Award for the Best Undergraduate Oral Presentation in Inorganic Chemistry
- CIC Award for the Best Undergraduate Poster Presentation in Inorganic Chemistry
- CIC Award for the Best Undergraduate Oral Presentation in Materials Chemistry
- CIC Award for the Best Undergraduate Poster Presentation in Materials Chemistry
- CIC Award for the Best Undergraduate Oral Presentation in Organic Chemistry
- CIC Award for the Best Undergraduate Poster Presentation in Organic Chemistry
- CIC Award for the Best Undergraduate Oral Presentation in Physical, Theoretical or Computational Chemistry
- CIC Award for the Best Undergraduate Poster Presentation in Physical, Theoretical or Computational Chemistry
- Best Graduate Oral Presentation
- Best Graduate Poster Presentation
- ACEmat Award in Computational Modeling of Materials
- E. Gordon Young Award for Best Pedagogical Graduate Oral Presentation
- Science Atlantic Science Communication Award
- Science Atlantic Undergraduate Research Award
- Murray Brooker Award for Best Undergraduate Oral or Poster Presentation in Chemical Education
- Best Overall Presentation by an Undergraduate Student
Main Schedule

Day 1 (Friday, May 24):

1:00 pm – 4:45 pm  Registration – KCIC Main Foyer
4:45 pm – 5:00 pm  Opening Remarks – KCIC Main Auditorium
5:00 pm – 6:00 pm  Guest Speaker: Dr. Peter W. Mullen – KCIC Main Auditorium
6:30 pm – 9:00 pm  Pizza and Trivia – The Axe Lounge (Open until 1 am)

Day 2 (Saturday, May 25):

8:00 am – 9:15 am  Breakfast – Wheelock Dining Hall
9:30 am – 10:30 am  Oral Presentations: Session 1 – KCIC Main Auditorium
10:30 am – 10:45 am  Snack Break – KCIC Garden Room
10:45 am – 11:45 am  Guest Speaker: Dr. Belinda Kemp – KCIC Main Auditorium
11:45 am – 12:45 pm  Lunch – Wheelock Dining Hall
1:00 pm – 2:50 pm  Poster Session/Grad Fair – Fountain Commons
3:00 pm – 3:15 pm  Snack Break – KCIC Garden Room
3:15 pm – 5:15 pm  Oral Presentations: Session 2 – KCIC Main Auditorium
5:15 pm – 6:15 pm  Science Atlantic Meeting – KCIC Basement Classroom
6:15 pm – 7:15 pm  Meeting 2 – KCIC Basement Classroom
7:15 pm  Leave for Wine Tour – In front of KCIC
7:30 pm – 8:45 pm  Wine Tour – Lightfoot and Wolfville Vineyards
8:45 pm  Depart Lightfoot and Wolfville Vineyards
9:00 pm  Arrive at KCIC

Day 3 (Sunday, May 26):

8:00 am – 8:45 am  Breakfast – Wheelock Dining Hall
9:00 am – 10:30 am  Oral Presentations: Session 3 – KCIC Main Auditorium
10:30 am – 10:45 am  Snack Break – KCIC Garden Room
10:45 am – 11:45 am  Oral Presentations: Session 4 – KCIC Main Auditorium
11:45 am – 12:45 pm  Lunch – Wheelock Dining Hall
12:45 pm – 3:00 pm  Oral Presentations: Session 5 – KCIC Main Auditorium
3:00 pm – 3:15 pm  Snack Break – KCIC Garden Room
3:15 pm – 5:15 pm  Oral Presentations: Session 6 – KCIC Main Auditorium
5:15 pm – 5:45 pm  Judges Meeting – KCIC Basement Classroom
6:45 pm – 9:30 pm  Banquet – Fountain Commons
**Student Presentation Schedule**

**Saturday, May 25, 2019**

<table>
<thead>
<tr>
<th>Session 1</th>
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<tbody>
<tr>
<td>9:30 am</td>
<td>AN-U-1</td>
<td>Ariana Joseph, SMU</td>
</tr>
<tr>
<td>9:45 am</td>
<td>AN-U-2</td>
<td>Kaleigh McLeod, SMU</td>
</tr>
<tr>
<td>10:00 am</td>
<td>AN-G-1</td>
<td>Anayet Kabir, UPEI</td>
</tr>
<tr>
<td>10:15 am</td>
<td>MA-U-1</td>
<td>Kuljit Kaur, CBU</td>
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<thead>
<tr>
<th>Session 2</th>
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<tbody>
<tr>
<td>3:15 pm</td>
<td>MA-U-2</td>
<td>Evan Connors, MUN</td>
</tr>
<tr>
<td>3:30 pm</td>
<td>MA-U-3</td>
<td>Scott Young, DAL</td>
</tr>
<tr>
<td>3:45 pm</td>
<td>MA-G-5</td>
<td>Sarah Martell, DAL</td>
</tr>
<tr>
<td>4:00 pm</td>
<td>MA-U-5</td>
<td>Sarah Clarke, MUN</td>
</tr>
<tr>
<td>4:15 pm</td>
<td>MA-G-1</td>
<td>Tianjun Zhang, DAL</td>
</tr>
<tr>
<td>4:30 pm</td>
<td>MA-G-2</td>
<td>Jeffrey Simmons, DAL</td>
</tr>
<tr>
<td>4:45 pm</td>
<td>MA-G-3</td>
<td>Dreenan Shea, STFX</td>
</tr>
<tr>
<td>5:00 pm</td>
<td>MA-G-4</td>
<td>Ziyi Chen, DAL</td>
</tr>
</tbody>
</table>

**Sunday, May 26, 2019**

<table>
<thead>
<tr>
<th>Session 3</th>
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<tbody>
<tr>
<td>9:00 am</td>
<td>BI-U-1</td>
<td>Jennifer Kolwich, SMU</td>
</tr>
<tr>
<td>9:15 am</td>
<td>BI-U-2</td>
<td>Kaitlyn Blatt-Jamnaat, SMU</td>
</tr>
<tr>
<td>9:30 am</td>
<td>BI-U-3</td>
<td>Prashansa Kooshna, SMU</td>
</tr>
<tr>
<td>9:45 am</td>
<td>BI-G-1</td>
<td>Brandon Logan, SMU</td>
</tr>
<tr>
<td>10:00 am</td>
<td>IN-U-1</td>
<td>Ben Nadeau, UNBF</td>
</tr>
<tr>
<td>10:15 am</td>
<td>OR-G-5</td>
<td>Michael Beh, DAL</td>
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<thead>
<tr>
<th>Session 4</th>
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<tbody>
<tr>
<td>10:45 am</td>
<td>IN-U-2</td>
<td>Brandon Frenette, UNBF</td>
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<tr>
<td>11:00 am</td>
<td>IN-G-1</td>
<td>Dylan Hale, DAL</td>
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<tr>
<td>11:15 am</td>
<td>OR-U-1</td>
<td>Jun Luo, ACADIA</td>
</tr>
<tr>
<td>11:30 am</td>
<td>OR-U-2</td>
<td>Kirkland Lockyer, MUN</td>
</tr>
<tr>
<td>Time</td>
<td>Session</td>
<td>Speaker</td>
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<tr>
<td>1:00 pm</td>
<td>OR-U-3</td>
<td>Liam Payne</td>
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<tr>
<td>1:15 pm</td>
<td>OR-U-4</td>
<td>Michel Deschenes</td>
</tr>
<tr>
<td>1:30 pm</td>
<td>OR-U-5</td>
<td>Ryan Warren</td>
</tr>
<tr>
<td>1:45 pm</td>
<td>OR-G-1</td>
<td>Shayan Azher</td>
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<tr>
<td>2:00 pm</td>
<td>OR-G-2</td>
<td>Matthew Laprade</td>
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<tr>
<td>2:15 pm</td>
<td>OR-G-3</td>
<td>Blake Huchenski</td>
</tr>
<tr>
<td>2:30 pm</td>
<td>OR-G-4</td>
<td>Erin Welsh</td>
</tr>
<tr>
<td>2:45 pm</td>
<td>PC-U-1</td>
<td>Alex Hebert</td>
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<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker</th>
<th>University</th>
</tr>
</thead>
<tbody>
<tr>
<td>3:15 pm</td>
<td>PC-U-2</td>
<td>Christopher Qiu</td>
<td>MUN</td>
</tr>
<tr>
<td>3:30 pm</td>
<td>PC-U-3</td>
<td>Chad Turner</td>
<td>UPEI</td>
</tr>
<tr>
<td>3:45 pm</td>
<td>PC-U-4</td>
<td>Chun Keat Khor</td>
<td>UNBF</td>
</tr>
<tr>
<td>4:00 pm</td>
<td>PC-U-5</td>
<td>Holly Studzinski</td>
<td>UPEI</td>
</tr>
<tr>
<td>4:15 pm</td>
<td>PC-U-6</td>
<td>Timara Uhlig</td>
<td>UPEI</td>
</tr>
<tr>
<td>4:30 pm</td>
<td>PC-G-1</td>
<td>Andrew Walsh</td>
<td>DAL</td>
</tr>
<tr>
<td>4:45 pm</td>
<td>PC-G-2</td>
<td>David Morris</td>
<td>DAL</td>
</tr>
<tr>
<td>5:00 pm</td>
<td>PC-G-3</td>
<td>David Do</td>
<td>DAL</td>
</tr>
</tbody>
</table>

AN = Analytical  
BI = Biochemical  
IN = Inorganic  
MA = Materials  
OR = Organic  
PC = Physical/Computational  
U = Undergraduate  
G = Graduate  
P = Poster  

ACADIA = Acadia University  
CBU = Cape Breton University  
DAL = Dalhousie University  
MUN = Memorial University  
MTA = Mount Allison University  
SMU = Saint Mary’s University  
STFX = St. Francis Xavier University  
UNBF = University of New Brunswick - Fredericton  
UPEI = University of Prince Edward Island
## Poster Presentations

<table>
<thead>
<tr>
<th>Poster Session</th>
<th>Name</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>AN-UP-1</td>
<td>Clarke Brown</td>
<td>DAL</td>
</tr>
<tr>
<td>BI-UP-1</td>
<td>Sarah Boudreau</td>
<td>CBU</td>
</tr>
<tr>
<td>PC-UP-1</td>
<td>Kennedy Brittain</td>
<td>SMU</td>
</tr>
<tr>
<td>OR-UP-1</td>
<td>Jacob Campbell</td>
<td>SMU</td>
</tr>
<tr>
<td>IN-UP-1</td>
<td>Jordan Conrad</td>
<td>UNBF</td>
</tr>
<tr>
<td>AN-UP-2</td>
<td>Samantha Corkum</td>
<td>DAL</td>
</tr>
<tr>
<td>BI-UP-2</td>
<td>Julie Anne Dayrit</td>
<td>SMU</td>
</tr>
<tr>
<td>BI-GP-1</td>
<td>Abdurrahman Elajmi</td>
<td>SMU</td>
</tr>
<tr>
<td>BI-UP-3</td>
<td>Kaela Fraser</td>
<td>ACADIA</td>
</tr>
<tr>
<td>IN-UP-2</td>
<td>Tanner George</td>
<td>SMU</td>
</tr>
<tr>
<td>MA-UP-1</td>
<td>Elvin Girineza</td>
<td>STFX</td>
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<td>OR-UP-2</td>
<td>Jacob Hoare</td>
<td>SMU</td>
</tr>
<tr>
<td>IN-GP-1</td>
<td>Helia Hollenhorst</td>
<td>DAL</td>
</tr>
<tr>
<td>AN-UP-3</td>
<td>Toren Hynes</td>
<td>DAL</td>
</tr>
<tr>
<td>IN-UP-3</td>
<td>Dakshita Jagota</td>
<td>MUN</td>
</tr>
<tr>
<td>AN-UP-2</td>
<td>Alysson Jones</td>
<td>DAL</td>
</tr>
<tr>
<td>MA-UP-2</td>
<td>Nikita Kenney</td>
<td>STFX</td>
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<tr>
<td>MA-UP-3</td>
<td>Annabelle Kilham</td>
<td>MTA</td>
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<tr>
<td>IN-GP-2</td>
<td>Marcus Kindervater</td>
<td>DAL</td>
</tr>
<tr>
<td>PC-UP-2</td>
<td>Shannon MacLennan</td>
<td>STFX</td>
</tr>
<tr>
<td>MA-UP-4</td>
<td>Tiffany MacLennan</td>
<td>STFX</td>
</tr>
<tr>
<td>AN-UP-6</td>
<td>Harrison Max</td>
<td>DAL</td>
</tr>
<tr>
<td>OR-UP-3</td>
<td>Jenna McNutt</td>
<td>ACADIA</td>
</tr>
<tr>
<td>PC-UP-3</td>
<td>Tara Misener</td>
<td>UPEI</td>
</tr>
<tr>
<td>AN-UP-4</td>
<td>Soraya Moore</td>
<td>MUN</td>
</tr>
<tr>
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Abstracts: Guest Speakers
Dr. Peter W. Mullen

The Forensic Toxicology of Alcohol

This presentation will be an overview of the key, interesting pharmacological/toxicological aspects of alcohol (ethanol) including its measurement in body fluids in the context of Canadian Law.

Topics to be considered:

- Adverse outcomes related to alcohol use
- Canadian Law re. alcohol-impaired driving
- Pharmacodynamics (effects) & pharmacokinetics (disposition in the body over time) of alcohol
- Novel metabolites of alcohol
- Breath measurements of alcohol
- Biomarkers to determine alcohol use
- Alcohol in body fluids, postmortem
- Wine: Alcohol plus?
The application of chemistry in winemaking

The application of the principles and theories of chemistry throughout the winemaking process, during the grape ripening stages through to finished wine. The chemical analysis used by winemakers, the reasons why specific parameters in juice and wine are measured, and the importance of the chemical composition of wine will be explored as she takes you on a chemical journey through the winemaking process from the grapevine to the bottle.
Abstracts: Oral Presentations
AN-U-1
Ariana Joseph
Saint Mary’s University

Polarization-Resolved Second Harmonic Generation Microscopy: A Novel Technique for Differentiation of Tumour Tissue
Ariana Joseph, Richard Cisek, Brian C. Wilson, Virginijus Barzda, and Danielle Tokarz*

The deregulation of cell division and consequent disorganization of the cellular microenvironment are characteristic of cancer initiation and proliferation. While statistics show that cancer rates generally increase with age, the disease is not limited to a specific age, race or ethnicity.\textsuperscript{1} Cancer misdiagnoses are one of the numerous factors influencing cancer mortality rates. The misdiagnosis rate ranges from 10-20% and almost doubles in aggressive cancer types such as pancreatic cancer.\textsuperscript{2} Automated cancer detection has the potential to detect minute changes in normal tissue below the current threshold of staining detection methods, resulting in earlier detection, more accurate diagnosis and reduced mortality rates. In the current research, differences in the collagen ultrastructure of the extracellular matrix in normal and cancerous pancreatic tissue were investigated using polarization-resolved second harmonic generation (SHG) microscopy. The polarization technique, polarization-in, polarization-out (PIPO), was utilized to obtain the second-order nonlinear optical susceptibility tensor component ratios: $\chi^{(2)}_{zzz}/\chi^{(2)}_{zxx}$ and $\chi^{(2)}_{xyz}/\chi^{(2)}_{zxx}$, as well as the degree of linear polarization (DOLP) from fits of the PIPO SHG data assuming C6 symmetry. A total of 98 tissue samples from 22 individuals were obtained from the tissue bank (Toronto General Hospital). Regions containing advanced adenocarcinoma (47 samples, 9 individuals), as well as normal sections (51 samples, 13 individuals) from lobular, parenchymal and periductal regions of the pancreas were investigated. Statistically-significant differences were observed in the distribution width of the $\chi^{(2)}_{xyz}/\chi^{(2)}_{zxx}$ values, as well as in average $\chi^{(2)}_{zzz}/\chi^{(2)}_{zxx}$ and DOLP values for normal and tumour pancreatic tissues, demonstrating that the technique could potentially be integrated into the field of histopathology.
AN-U-2
Kaleigh McLeod
Saint Mary’s University

On the origin of electrochemical surface-enhanced Raman spectroscopy (EC-SERS) signals for bacterial samples and electrode functionalization strategies
Kaleigh McLeod, Taylor Lynk, Christa L. Brosseau*, and Clarissa S. Sit*

Pathogenic bacteria is of large concern in many areas such as in clinical applications, food industry, and water supply. The field of point-of-need screening does not currently have a rapid, reliable and cost-effective method for the detection of bacteria. Surface-enhanced Raman spectroscopy (SERS) has been increasingly put forward as a possible option for the detection of biological species due to the rich vibrational modes that they produce. Electrochemical surface-enhanced Raman spectroscopy (EC-SERS) has not yet been explored in great detail for the detection of bacteria but has the potential to improve upon the sensitivity of SERS by applying a potential. Recently, there has been confusion surrounding the source of Raman bacterial peaks. This work shows the origin of these bacterial peaks is the result of small metabolites in solution released by bacteria under stress conditions. Additionally, a route of electrode functionalization is presented which shows the potential to increase bacterial adhesion to the silver nanoparticles.

Diatoms loaded self-assembled nanomaterial for co-delivery of drugs

Anayet Kabir and Marya Ahmed*

A rapidly expanding field that utilizes nature-inspired materials to create novel and functional biomimetics is known as “Biotemplating”. The diatomaceous earth is an exceptional template for drug delivery applications, owing largely to its highly-ordered pores, large surface area, species specific architecture, and flexibility for surface modifications. Diatomaceous earth have been studied in a wide range of biomedical applications but their potential as the next frontier of drug delivery has yet to be fully exploited. Diatoms are porous silica-based materials obtained from single cell photosynthetic algae. We are evaluating the potential of diatomaceous earth (DE) microparticles for the duel delivery of drugs as cancer therapeutics. The study described the self-assembly of adamantine modified diatomaceous earth in β-cyclodextrin architecture to prepare thixotropic gels of varying mechanical properties. The gels produced exhibit excelled drug absorption capacity and colloidal stability under different pH. The co-encapsulation of drugs in diatomaceous earth containing thixotropic materials is studied and their in vitro anticancer activities are evaluated.
MA-U-1
Kuljit Kaur
Cape Breton University

Development of Cost-Efficient Hybrid Biochar-Hydrogel Based Water Purification System
Kuljit Kaur, Stephanie MacQuarrie*, and Jegatha Esther*

In India, 21 percent of communicable diseases are linked to unsafe water and the lack of hygiene practices. Furthermore, more than 500 children under the age of five die each day from diarrhea. Also, more than 300 of 800 million people in Africa are impact by unsafe water whereas 115 people in Africa die every hour from typhoid, cholera, dysentery and diarrhea. There is an immediate need for the cost-efficient water purification especially in remote areas. Here we investigate the use of forestry residue charcoal as a filtration media. We have shown that the charcoal is effective to reduce the hardness of the water and neutralizing its pH. The morphology of the charcoal is critical for the flow system applications. We have shown that implementing various concentrations of charcoal into bio-polymer beads generated a media that is capable of adsorption of dyes, removal of ppm levels of sulfates and Iron and reduction in turbidity.
MA-U-2
Evan Connors
Memorial University of Newfoundland

Synthesis and Study of Gold Nanoparticles on a Liquid Interface for Thin Film Deposition

Evan Connors, Silvana Pereira, Yunfei Wang, Yuming Zhao, and Erika Merschrod*

Gold nanoparticle thin films are well known as effective substrates for use in surface enhanced Raman spectroscopy (SERS). Even with the wide use of Au-NP thin films as SERS substrates, the NPs are commonly synthesized through the multistep synthesis of capping of gold with dodecanethiol. We are working on developing Au-NPs thin films through a novel synthesis of the nanoparticles on a liquid interface capping them with a dithiafulvene (DTF) derivative allowing direct deposition on solid surfaces. The DTF capped Au-NP were prepared and observed by UV-Vis spectroscopy. The NPs drop casted were observed with Raman spectroscopy and atomic force spectroscopy (AFM). The film was then prepared by Langmuir-Blodgett film. The film, deposited on a quartz crystal microbalance (QCM), was observed by AFM and SEM. Understanding the size of the nanoparticles and how the film arranges on the QCM will allow better deposition of the films therefore allowing the fabrication of SERS substrates.
Additive Inactive Components in Silicon-Iron Alloy Negative Electrode Material for Advanced Lithium-ion Cells
Scott Young and Mark Obrovac*

Lithium-ion batteries (LIB) have an increasing importance in society today where renewable energy sources will count on their reliable energy storage to reduce the need of fossil fuel consumption. A goal of research in lithium-ion batteries is to help the ecosystem by allowing the utilization and storage of renewable energy while also allowing smartphones/tablets to last longer on a single charge.

Advances in Lithium-ion batteries are needed to better utilize their energy storage for applications such as fully electric vehicles (EVs) and the renewable energy grid. One field of research to enhance lithium-ion cell capacity is silicon (Si) based negative electrode materials. An increase in capacity would allow EVs to travel further distances on a single charge as well as many other applications. However, there are drawbacks to utilizing Si-based electrodes, and one of the most challenging obstacles is volume expansion.

When a Si negative electrode is lithiated, the Si expands by 280%. Such a drastic change in volume during cell cycling causes the structure to decay leading to poor cell performance. In this research, Si is alloyed with an electrochemically inactive material such as iron (Fe) to control volume expansion. This is an important discovery because it is counter intuitive to give valuable space in the negative electrode to atoms that are inactive to the cells processes. This research is looking at developing Si-inactive alloy materials with additive inactive components that benefits the performance of the lithium ion cell.
Silicon is a desirable element to work with since it is the second most abundant element in the Earth’s crust and biocompatible. Because of these attractive properties, nanostructured mesoporous silicon has been explored as a battery anode material, photocatalyst, sensor, and drug delivery vehicle [1]. In the recent years, hydrogen terminated mesoporous silicon have also emerged as a reactive precursor in CO$_2$ [2] and phosphine [3] reduction. This presentation will highlight new reactivity of hydrogen terminated mesoporous silicon nanoparticles. A modified magnesiothermic reduction method was developed to prepare porous silicon nanoparticles with surface area $> 450$ m$^2$/g. Various etching procedures were investigated to maximize the number of hydrogen moieties on the silicon surface which was quantified using NMR. The etching process was optimized as function of reaction time and amounts of nitric acid and hydrofluoric acid added. Hydrogen terminated mesoporous silicon nanoparticles possessing highest surface area were investigated for photocatalytic water splitting.
MA-U-5
Sarah Clarke
Memorial University of Newfoundland

Preparation and Analysis of Cobalt Ferrite Nanoparticles for SERS Detection of Polycyclic Aromatic Hydrocarbons

Sarah Clarke, Stephanie M. Gallant, Liudmila Strelnikova, and Erika F. Merschrod*

The carcinogenic nature of polycyclic aromatic hydrocarbons (PAHs), as well as their prevalence in the environment, make them an important class of molecules to detect. Municipal and industrial wastewater, oil spills, and fuel combustion are all ways for PAHs to enter the environment. Although they appear in low concentrations, they can bioaccumulate in wildlife and cause the deterioration of ecosystems. The focus of this work is to develop new composite surface-enhanced Raman spectroscopy (SERS) substrates for detecting low concentrations of PAHs. Cobalt ferrite NPs are cheap and simple to prepare and were synthesized using a one-pot precipitation method in air. These NPs were then characterized with a variety of methods such as powder X-ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, and energy dispersive X-ray spectroscopy (EDS). Once synthesized, these NPs are then layered over an annealed gold thin film to form a composite substrate for fast and sensitive PAH detection.
Building highly active Ti-containing zeolites through structural modification
Tianjun Zhang, Zhang Peng

As one of the most important members of the zeolite family, Ti-containing zeolites have scientific and technological interest due to the excellent properties in the environmentally-benign selective epoxidation of alkenes to epoxides. However, the sole micropore in conventional titanium silicate greatly inhibits the intracrystalline diffusion and adsorption of bulky molecules on the accessible active sites, thus limiting its applications in petrochemical processing and fine chemicals. Herein, we successfully develop a synthetic strategy to construct hierarchical Ti-containing zeolites with MFI and MWW topologies by using a rotational crystallization method. The obtained catalyst show excellent catalytic activity for the epoxidation of alkenes. Through further characterization of these Ti-containing zeolites with a library of techniques, their structure-property relationships are revealed.
MA-G-2
Jeffrey Simmons
Dalhousie University

Exploring the Structural and Mechanical Properties of Recombinant Spider Pyriform Silk

Jeffrey Simmons, Lingling Xu, Isaac Bridge, and Jan K. Rainey

Spider silks are biomaterials mechanically comparable to high strength steel and Kevlar, and used for many diverse adaptations by spiders. The orb-weaving spiders produce up to seven distinct types of silk, including pyriform silk. In nature, pyriform silk is spun as part of a glue-coated attachment disc, connecting web silks to disparate materials and, putatively, to each other. Even though this silk fills a critical role in web formation, neither the structural nor mechanical properties of pyriform silk have been widely investigated. Based on the central pyriform silk repetitive domain from *Argiope argentata*, we have successfully engineered recombinant pyriform silk-based proteins. Using these proteins to spin silk fibres, we have shown that recombinant pyriform silk is both strong and extensible, in contrast to mechanical extremes of strength at the expense of extensibility or vice versa seen in most silks. To develop the structure-function relationship for this silk, we are first performing solution-state structural studies of these recombinant silk proteins. Far-UV circular dichroism spectroscopy implies a predominantly α-helical structure in solution over a range of temperatures and independent of the number of repetitive units connected together. Distinct regions of order and disorder in the repetitive domain are implied based upon degrees of nuclear magnetic resonance (NMR) spectroscopy chemical shift dispersion correlated to the sign of $^1$H-$^{15}$N nuclear Overhauser effect enhancements. This is consistent with a sequence that has segregated structured and disordered/polyproline-II regions. Moving forward, elucidation of structural transitions between the soluble and fibrous states is being targeted.
Contamination of the global water ways by industrial waste is a pressing environmental issue. Furthermore, global availability of clean drinking water remains a struggle. Many common drugs, such as estradiol, are present in water samples and have been proven to bioaccumulate within human tissues. To date, research in this area has been focused on the use of light as of means of “photodegrading” these aqueous pollutants. Titanium dioxide (TiO$_2$) is a popular semiconductor due to its low cost and high photostability but is plagued with many shortcomings: (i) requiring high energy UV light activation and (ii) complete removal of the solid is quite difficult due to its small particle size (~30 nm). The latter is of large concern due to the potential contamination of the watershed with fine particulate matter. Potassium niobium oxide perovskites (KNbO$_3$) have similar light-active properties to TiO$_2$ but hold a clear advantage due to larger particle size (~1 mm) allowing for more facile catalyst recovery. Decoration of the KNbO$_3$ surface with Au nanospheres (AuNP; $\lambda_{\text{max}} = 530$ nm) can improve upon the light-induced activity of the solid and, most importantly, increase the response of the solid to favour lower energy (visible) light. The ability of the AuNP/KNbO$_3$ composite to facilitate the photodegradation of estradiol will be discussed. Several parameters will be examined in an effort to maximize the efficiency of the photodegradation route, including the influence of environmental pH, as well as a variety of photocatalyst and pollutant concentrations.
MA-G-4
Ziyi Chen
Dalhousie University

Structure and bonding properties of some silver and alloy nanoclusters by X-ray spectroscopy
Ziyi Chen and Peng Zhang*

X-ray spectroscopy is a good tool for study the structure and bonding properties of nanoclusters. Nanoclusters with an exact number of atoms have intriguing properties and can be applied in many fields. In this presentation, the study of some nanoclusters in terms of their structural and bonding properties by X-ray spectroscopy techniques such as X-ray absorption spectroscopy and X-ray photoelectron spectroscopy will be presented. Systems of interest include some doped and undoped atomically precise silver nanoclusters. It will be demonstrated that the structural and property changes between doping and non-doping clusters can be sensitively captured by X-ray spectroscopy techniques. The information obtained from the X-ray techniques will also be useful to more thoroughly understand the stability and structural control of those nanoclusters.
BI-U-1

Jennifer Kolwich
Saint Mary’s University

Discovery and investigation of fungus-derived antimicrobial compounds with activity against Pseudogymnoascus destructans, the causative agent of bat White-nose Syndrome

Jennifer Kolwich, Lindsay Donovan, and Clarissa Sit*

White-nose syndrome (WNS) is an emergent disease in North American bat populations. Since the first documented case in New York just over a decade ago, WNS has spread to 33 states and 7 provinces, leading to population decreases of 90-100% in some sites.¹,² The causative agent of WNS was determined to be the fungal pathogen Pseudogymnoascus destructans (Pd).²,³ Recent studies that have had success at treating WNS utilize the status of Pd as an invasive species in the skin microbiome of North American bats; they have found that micro-ecological defenses of pre-existing cutaneous specimens could be the key in reducing the effect of the fungus. With this in mind, we have isolated and purified samples of cutaneous microbes from a colony of big brown bats. These purified strains have undergone pairwise assays against Pd and three closely related Pseudogymnoascus species to test for inhibitory activity. The metabolites of biologically active strains were extracted and tested directly for antimicrobial activity. Potent biological activity has been observed and is being investigated to determine the nature of the activity and the identity of the metabolites.

A Happy Accident: Microbial Volatiles for Plant Defense
Kaitlyn Blatt-Janmaat and Clarissa Sit*

Plant pathogens and pests can impact food security by damaging crops and reducing yields. In future years, the variety and abundance of these organisms are expected to increase due to the changing climate. As a result, farmers rely heavily on chemical control agents such as herbicides, pesticides, and fungicides. While these treatments are effective, concerns over both human and environmental health have been raised due to the high frequency of their use. As such, additional methods of pathogen control have been investigated such as intercropping and biocontrol agents. One interesting avenue of investigation is the use of plant growth promoting bacteria for growth enhancement and pathogen suppression. Plant associated microbes can produce a variety of metabolites that directly benefit the host and they can also act as an external immune system by producing antimicrobial agents. These compounds can be large molecules such as peptides or lipids, or small volatile compounds. In this work, volatile inhibition of a suspected plant pathogen by plant derived bacteria was observed and explored with HS-SPME-GC-MS. Headspace profiles of multiple strains were compared in an attempt to determine which compounds demonstrated antifungal activity. Implications and further applications of this work will be discussed.
Nova Scotian Honeybees as potential sources for antimicrobial compounds against American Foulbrood disease
Prashansa Kooshna, Morgan Crosby, Abdurrahman El Ajmi, and Clarissa Sit*

Honeybees, *Apis mellifera*, are important pollinators in our ecosystem as well as in agricultural industry. However, there has been a global decline in honeybee populations in recent years due to various factors. Contagious diseases such as American Foulbrood (AFB), caused by *Paenibacillus larvae*, can significantly reduce honeybee populations. From previous studies, various microbes from apiarian sources were found to inhibit the pathogen. Our study involves looking for microbes found in Nova Scotian honeybees that have inhibitory effects against *P. larvae*. So far, 200+ isolates have been obtained from our samples of beehive swabs as well as the exteriors of the bees. Currently, these isolates are being screened for inhibition against *P. larvae* using pairwise assays. Our goal is to extract and characterize secondary metabolites from the microbes that exhibit activity, using HPLC and LC/MS.
Investigating soil microbial biodiversity and how it impacts natural wine fermentation
Brandon Logan and Clarissa Sit*

Wine has been around for many millennia. Current conventional winemaking relies on microbial starting cultures for fermentation, as opposed to historical methods which were dependent on spontaneous fermentations. However, the latter method of winemaking is re-emerging in a trend known as natural fermentations or natural wine. This method relies on naturally occurring yeast and microbes found on the grapes to conduct fermentation. Evidence suggests that the soil acts as a reservoir for plant microbiological communities\textsuperscript{1}, and therefore supports the idea that microbes found on grapes originate from the soil. This research project is an exploratory investigation into the effect soil microbes have on natural wine fermentations. To investigate this phenomenon, metagenomics of soil microbes and their metabolomics must be considered. Along with soil samples, swabs of various plant tissues have been collected from an array of Nova Scotian vineyards in an attempt to isolate and identify microbes potentially affecting the wines. Microvinifications will be carried out using single species of microbes and analyzed by various analytical techniques to understand what role they may play in the overall process. Using this information, we hope to correlate several flavours or aromas with specific microbes. This information may be useful to vineyards and winemakers interested in exploiting natural ferments, and may have implications in other fields such as brewing.

IN-U-1
Ben Nadeau
University of New Brunswick—Fredericton

Detection of DPA in Bacillus subtilis endospores using a Europium(III) complex
Ben Nadeau and Barry Blight*

A new luminescent Eu(III) complex was synthesized and tested as a ‘turn-off’ sensor for a Bacillus anthracis biomarker, dipicolinic acid (DPA). This work presents ideas and developments towards functionalized terpyridine ligands for the synthesis of solid-state Eu(III) polymer sensors. The synthesized Eu(III) complexes were soluble in organic solvents (THF, MeOH) and were used at micromolar concentrations for detection of DPA in lab grown Bacillus subtilis endospores. The Eu(III) complexes successfully detected the extracted and isolated DPA from B. subtilis endospores and luminescent quenching was observed after titration studies using both commercial DPA and treated B. subtilis endospores, further confirming the ‘turn-off’ sensing abilities of Eu(III) systems.
Synthesis of (Poly)Pyrroles: Bridging the Gap with Sulfur
Michael Beh and Alison Thompson*

The preparation of sulfur-bridged pyrroles without the use of sulfur dichloride was explored. Two alternative syntheses have been developed, which, with further effort, have the potential to allow easier access to sulfide-bridged pyrroles. The first example of electrophilic aromatic substitution of pyrrole using thionyl chloride to produce a sulfide-bridged dipyrrole is discussed, including a mechanism for the reductive reaction. Further, the first example of a sulfide-bridged dipyrrole prepared via nucleophilic aromatic substitution of an α-chlorinated pyrrole with sodium sulfide nonahydrate is discussed, as well as attempts to make sulfide-bridged tetrapyrrroles.
Brandon Frenette
University of New Brunswick—Fredericton

The synthesis of tetra(iminophosphorano)-substituted bispyridinylidenes; organic super-electron donors with record-breaking redox potentials

Brandon Frenette, Nadine Arseneault, Sarah Walker, and C. Adam Dyker*

Organic electron donors can be useful alternatives to metal-based reductants, in some cases offering milder reaction conditions or interesting selectivity. Currently, their utility as reagents is limited by their weaker redox potentials compared to metals. Developing stronger organic reductants is thus necessary to broaden their applicability. Recent progress has come in the form of bispyridinylidenes (BPYs) – strong organic electron donors with redox potentials that are highly-tunable by changing their substituents.¹² The superb π-electron donating ability of iminophosphorano substituents (R₃P=N-, R = phenyl, cyclohexyl) has been exploited to synthesize a series of novel BPYs. These reducing agents are the strongest neutral organic two-electron donors yet realised. This presentation will outline the synthesis of these novel BPYs. The highly-reactive electron donors have been characterized in situ by NMR and cyclic voltammetry, and isolated as bipyridinium salts for further characterization. The air- and moisture-stable precursors are readily prepared in multi-gram quantities with good yields and can be used to easily generate the electron donors in situ via deprotonation.

IN-G-1
Dylan Hale
Dalhousie University

Bis(phosphino)silyl Co(I) Pincer Complexes for the Catalytic Hydrogenation of Alkenes
Dylan Hale and Laura Turculet*

Catalysts that utilize first row transition metals in lieu of their heavier second and third row congeners have recently attracted significant attention due to the relatively high abundance and low cost of the first row metals. While such sustainable catalysts are being utilized for a variety of applications, research in the Turculet group has focused on the catalytic reduction of unsaturated substrates. In this regard, catalysts capable of performing direct alkene hydrogenation with H₂ are especially attractive due to the inherent atom economy of the reaction, which generates little to no waste. Previous work in the Turculet group has shown that bis(phosphino)silyl (PSiP) supported Fe[1] and Co[2] complexes can facilitate alkene hydrogenation through generation of metal hydrides, with the readily isolated complex (PSiP)FeH(N₂)₂ proving to be a highly effective, easily manipulated precatalyst for the hydrogenation of a range of terminal and multiply-substituted alkenes. In an effort to access increasingly effective first row metal catalysts for such transformations, this presentation will focus on the development of new low-coordinate (PSiP)Co(I) complexes that can function as pre-catalysts for the direct hydrogenation of a wide range of alkene substrates under exceptionally mild conditions. Details of our experimental and computational investigation of this reactivity will be presented.

1. Murphy, L. J.; Ferguson, M. J.; McDonald, R.; Lumsden, M. D.; Turculet, L. Organometallics, 2018, 37, 4814–4826.
OR-U-1
Jun Luo
Acadia University

Green synthesis of novel naphthalene-based 14-aza-12-oxasteroid analogues
Jun Luo and Amitabh Jha*

Polyheterocyclic frameworks, such as steroids, are very important moieties for the construction of biologically and pharmaceutically relevant molecules. But synthesis of these structurally complex molecules in a short route from readily available starting materials is a challenge in the field of organic chemistry and therefore is widely being investigated. Here, a transition metal-free four-step synthetic pathway was developed to produce tetracyclic heterosteroid compounds, starting with 2-naphthols. After conversion to 2-naphthylamines via the Burcherer reaction, acetylation via the Sugasawa reaction and reduction using borohydride, the resulting 1-(1-hydroxyethyl)-2-aminonaphthalenes underwent double dehydrations and double intramolecular cyclisation with oxo-acids for a one-pot formation of a C-N bond, a C-O bond and an amide bond in tandem. In total, 6 novel 14-aza-12-oxasteroid analogues were synthesised with characterisation through $^1$H and $^{13}$C{$^1$H} NMR spectroscopies; ESI-HRMS was also conducted on several intermediates and final compounds to determine their exact masses.
Progress Towards the Synthesis of (4S,5S)-4,5-dihydroxy[8](2,7)pyrenophane

Kirklin Lockyer and Graham Bodwell*

Since the first report of anti-[2.2]metacyclophane by Pelligrin¹ in 1899, cyclophanes have cemented themselves as fascinating targets for organic synthesis. Their synthetic complexity continues to grow as researchers seek to incorporate different functionality, more complicated bridges and larger polycyclic aromatic hydrocarbons into their cyclophanes. Pyrenophanes are a class of cyclophane which incorporates a pyrene moiety within its structure. These systems have been an area of ongoing research in the Bodwell group for decades. This research project seeks to build on earlier work in the group aimed at the synthesis of a chiral $C_2$-symmetric [8](2,7)pyrenophane-diol, specifically (4S,5S)-4,5-dihydroxy[8](2,7)pyrenophane. While chiral pyrenophanes have been synthesized in the past by the Bodwell group, their chirality stemmed from the planar chirality caused by the positioning cyclophane bridge.² The interesting aspect of the target [8](2,7)pyrenophane-diol is its chirality is instead imparted by the stereogenic centres on the bridge. To ensure high enantiomeric purity in the final product, the chiral pool was utilized. While the synthesis of (4S,5S)-4,5-dihydroxy[8](2,7)pyrenophane remains elusive, progress has been made through the testing of different strategies for making the key connection between the bridge and the two arene units that will eventually form the pyrene moiety.

Figure 1: The structure of (4S,5S)-4,5-dihydroxy[8](2,7)pyrenophane

Liam Payne
University of Prince Edward Island

Laser Flash Photolysis Studies on Fluorophore Photoswitching Mechanisms
Liam Payne, Yasser Gidi, and Gonzalo Cosa*

Photoswitchable fluorophores have allowed the development of sub-diffraction resolution imaging techniques based on single molecule localization microscopy, such as stochastic optical reconstruction microscopy (STORM)\(^1\). Switching between ‘on’ and ‘off’ states allows the sequential localization of the centroid of the point spread function by fitting a 2D Gaussian function. In the presence of a primary thiol, the red-emitting cyanine dye Cy5 photoswitches to a dark state that can be recovered in its emissive state either thermally or upon exposure to UV, blue, or green light.\(^1-3\) While the chemical identity of the Cy5 dark state has been studied, its mechanism of formation and return to the emissive state remains to be elucidated. Understanding the mechanism by which Cy5 changes from an emissive state to a dark state is paramount in controlling dye photoswitching and the rational design of new photoswitchable dyes. Herein, we describe laser flash photolysis studies on Cy5 aimed at clarifying its photochemical and photophysical behavior.

OR-U-4
Michel Deschenes
University of New Brunswick—Fredericton

Towards a Novel (S)-2,2,6-trimethylcycloheptanone
Michel Deschenes and David MaGee*

Previous studies in the MaGee group have shown promise that himachalenes, a subclass of sesquitepenes, are of high interest in the field of aggregation pheromone research. In this project the synthesis (S)-2,2,6-trimethylcycloheptanone was attempted. To accomplish this, an optically enriched acyclic scaffold was synthesized to study the effects of a gem dimethyl group at the alpha position of the reaction site in the Dieckmann cyclisation. This study on the effect of this functionality is set to open numerous synthetic approaches for reaching the target bicyclic himachalene core of interest.
A new synthetic route to 1:2,13:14-dibenzo[2]paracyclo[2](2,7)pyrenophane-1,13-diene (1) was explored. It is expected that this new route will allow for the preparation of synthetically useful amounts of 1 as well as lay the groundwork for the synthesis of an extended system 2, which contains 2 basic units of pyrenophane 1. The sinusoidal topology of pyrenophane 2 makes it an interesting target due to its potentially unusual optical and spectroscopic properties. Retrosynthetically, 1 can be thought of in terms of three natural building blocks: a middle bis(boronic acid) or ester derivative (3), a corner dihalide unit (4), and an endcap (5), which brings the functionality needed to construct the bent pyrene systems. The focus of this work was primarily the manipulation of 5, with a goal of finding R groups that would allow for successive coupling reactions while simultaneously maintaining functionality to form the pyrenophane without undue synthetic manipulation. Several different strategies for the formation of pyrenophane 1 were envisioned depending upon the nature of R.
The amide linkage is one of the most important and well-recognized functional motifs in pharmaceutical chemistry.\(^1\) There are many methods available to synthetic chemists from which to build complexity around this well-known motif, thus allowing for the discovery of new compounds that may one day have far-reaching pharmaceutical and medicinal applications. One of these applications is the field of diagnostic imaging. Pyrene based materials have always attracted attention for their interesting fluorescence properties, as well as the role they may play in optoelectronic devices.\(^2\) It is therefore apparent that amides consisting of pyrene as a skeletal building block represent some interesting synthetic targets, particularly for application as tracers in bioimaging procedures. This presentation will highlight efforts towards the synthesis of a series of pyrene amides as well as progress towards the synthesis of a compound that may find application as a radiotracer, for early detection of prostate cancer.\(^3\)

Figure 1. Selection of some synthetic targets.

Highly unsaturated organic molecules possess interesting chemistry and properties, thanks in part to the hybridization of carbon atoms. The reactivity of unsaturated molecules can be enhanced by the presence of a carbocationic center. For instance, a carbocationic center adjacent to an alkyne is referred to as a propargyl carbocation, and its reactivity is expected to be increased. It is believed that the carbocation will withdraw electron density, causing the alkyne carbon (\(-\text{C}≡\text{C}-\text{C}^+\)) to become polarized and highly reactive. We have been able to isolate a stable propargyl carbocation, and have started to explore its chemistry.
OR-G-3
Blake Huckenski
Dalhousie University

Small molecule activation catalyzed by Bis-aminocyclopropenylidene derivatives
Blake Huckenski and Alex Speed*

The application of main group elements in catalysis has been rapidly growing in recent years. Elements such as phosphorus and boron have been utilized by our group to catalyze various reductions on unsaturated bonds. The bis-aminocyclopropenylidene and cyclopropenium ions represent an effective scaffold to construct catalysts as these complexes can often be prepared within a few synthetic steps. Herein we disclose the novel preparation of main group complexes as air stable precursors to catalytic systems, which can catalyze reductions, as well as their application in small molecule activation for catalysis.
The metal-free asymmetric catalytic reduction of unsaturated molecules is an emerging field of chemistry. Recently, our group demonstrated the asymmetric reduction of imines using enantioenriched N-heterocyclic phosphines, or NHPs, affording enantioenriched secondary amines.¹ One limiting factor in further optimization has been the ability to tune the catalyst due to the scarcity of commercially available enantioenriched primary amines. The work will disclose the synthesis of chiral amines and improved NHPs that increase the enantioselectivity in imine hydroboration reactions. This work reports the successful synthesis of multiple chiral NHPs through various methods and their performance in enantioselective reactions. Using our new catalysts we can access chiral amines of medicinal importance with efficiencies approaching or exceeding existing precious metal catalysts.

Gold nanoclusters are an emerging class of materials that show great promise in a wide variety of analytical, catalytic, and biomedical applications due to their unique optical properties. They exhibit single-photon and multi-photon absorptions, fluorescence, as well as excellent catalytic reactivity. To achieve their full potential, specifically in catalysis, it is important to understand how size, geometry, and ligand choice influence their electrodynamics.

A series of gold nanoclusters of various sizes (Au\textsubscript{18}–Au\textsubscript{144}) were prepared with thiolate protecting ligands. Raman spectroscopy was attempted on the most stable species of the clusters, Au\textsubscript{25}(SC\textsubscript{2}H\textsubscript{4}Ph)\textsubscript{18}. However, no peaks attributable to the nanocluster were observed. Femtosecond transient absorption spectroscopy was performed on each of the synthesized clusters and the kinetics of the excited-state relaxation were investigated. The majority of phenylethanethiolate-protected clusters exhibited a two-step relaxation decay, while the glutathionate-protected clusters exhibited a three-step decay, demonstrating the ligand effects on the excited-state dynamics of gold nanoclusters.

Finally, parallel factor analysis was applied to excitation-emission matrices of binary solutions of gold nanoclusters to develop a rapid technique to evaluate the monodispersity of nanocluster solutions. A qualitative, pass-fail, method of monodispersity evaluation was achieved, which could reduce the need for mass-spectrometry during cluster synthesis. The method also shows promise as a stand-alone evaluation of cluster solution monodispersity. However, more research is needed.
PC-U-2
Christopher Qiu
Memorial University of Newfoundland

DFT Investigations of the C-Si/B-Br Exchange Reaction Mechanism
Christopher Qiu, Christopher Flinn*, and Yuming Zhao*

The formation of C-B bonds has been an important field of research in the development of organic materials, one of which is the C-Si/B-Br exchange reaction.1-4 Despite its synthetic usefulness in the literature, the full mechanism has not yet been disclosed and its elucidation would yield insights into the development of further reactions and methodologies. This study investigated the mechanisms of the addition of BBr3 with trimethyl(phenyl)silane and para-trimethyl(toly)silane. A computational study using density functional theory (DFT) using the M06-2X/def2-SVP level of theory was employed to determine the energetics of possible ipso and electrophilic aromatic substitution pathways to determine the appropriate mechanism. Transition states and reactive intermediates were calculated and confirmed via intrinsic reaction coordinate (IRC) analysis. In addition to the computational work, 1H NMR studies of the phenyl and tolyl systems were also performed to confirm the validity of the DFT results and to observe the formation of possible side products. Results revealed that the mechanism proceeds through direct ipso substitution rather than electrophilic aromatic substitution, although the formation of by-products are also observed.
PC-U-3
Chad Turner
University of Prince Edward Island

A Theoretical Exploration of the Bent Bond Antiperiplanar Hypothesis using Electron Pair Distributions
Chad Turner and Jason Pearson

Advances in computational chemistry have allowed us to quantitate the behaviour of the ubiquitous electron pair by determining both the relative separation and absolute center-of-mass position of an individual electron pair. These tools, however, have not yet been used to probe into the nature of one of the most predominant theories of bonding in the past century and its recent extension: the Slater-Pauling bent bond model and the bent bond antiperiplanar hypothesis (BBAH). Here, we demonstrate the use of intracule and extracule densities to quantitively investigate the behaviour of lone pairs in systems that can be described by the Slater-Pauling bent bond model and BBAH. We found that the relative separation and center-of-mass distribution of lone pair electrons can be used to explain the overall stability of a molecule as it undergoes conformational changes by means of rotation about a defined dihedral angle. Furthermore, the energetically favourable conformations of a variety of molecules show direct links to the Slater-Pauling bent bond model and BBAH. We anticipate that this work will exhibit the usefulness of intracule and extracule calculations in investigating the nature of the chemical bond. Additionally, we believe that our findings could aide in a revival of the Slater-Pauling bent bond model as a descriptor for particular chemical systems.
Bispyridinylidenes (BPYs) are a type of homogenous, metal-free organic reducing agent that are readily oxidized by two-electrons to yield bipyridinium salts (bPyr). They can offer a wide range of redox potentials by switching the substituents that are attached to the BPY scaffold. For good selectivity in reducing a particular functional group over others, it is important to have a reducing agent of appropriate strength, which in turns requires methods for predicting redox potentials ($E_{1/2}$). The main goal of the project is to develop a correlation between $^{15}$N chemical shifts of pyridinium salts (Pyr) and $E_{1/2}$ of their corresponding bPyr/BPY couples. Hence, a number of different Pyr and their corresponding bPyr were prepared. The $^{15}$N chemical shifts of the Pyr were then determined using Hydrogen Nitrogen Heteronuclear Multiple Bond Correlation ($^1$H$^{15}$N-HMBC), a 2D NMR method, while the $E_{1/2}$ of their corresponding bPyr were determined using cyclic voltammetry (CV). The experimental methods and the predictive ability of $^{15}$N shifts of Pyr will be discussed in detail.
PC-U-5
Holly Studzinski
University of Prince Edward Island

Tetracyanoquinodimethane (TCNQ) as a Versatile Guest Probe of the Host Properties of Both Fluorescent and Non-Fluorescent Hosts

Holly Studzinski and Brian Wagner*

Tetracyanoquinodimethane (TCNQ) is a novel guest probe and its ability to act as a versatile guest probe for host inclusion studies of both fluorescent and non-fluorescent hosts makes it a very interesting molecule to study, with a wide range of potential applications. In this research project, the intrinsically fluorescent hosts cyclo[n](2,11)-teropyrenophanes (CnTP n=7-9) were studied. When host-guest inclusion complexes were investigated using fluorescence emission, it was concluded that all three host homologues formed 1:1 inclusion complexes with TCNQ. The binding constants for all three complexes were relatively small, but the fluorescence emission of the hosts was consistently suppressed upon inclusion, with C7TP, the smallest of the three hosts, showing the strongest binding. Results obtained are of significance due to the little information available about the CnTP hosts and TCNQ as a non-fluorescent probe. The more frequently studied non-fluorescent hosts, modified cyclodextrins, were also investigated in this study. These allowed TCNQ to be researched as a fluorescent guest probe in aqueous solutions. Results obtained from this research showed that an inclusion complex was formed only between TCNQ and the smallest modified cyclodextrin cavity size. Significant enhancement of fluorescence emission was obtained. Results also showed that in both types of hosts TCNQ had the greatest binding constant in the host cavities of the smallest size. This indicates that future research in this area should be conducted with hosts that have similar cavity sizes.
PC-U-6
Timara Uhlig
University of Prince Edward Island

Timara Uhlig and Brian D. Wagner*

Recently, a new family of host molecules known as pillar[n]arenes have been prepared and developed. Since their discovery, applications of this macrocycle have been investigated, however, there has been little research on the fluorescence studies of these hosts with respect to host-guest inclusion complexes. Interest in this host stems from its unique shape which differs from the more common hosts currently available. This host consists of repeating hydroquinone units connected by methylene bridges in the para position to give the macrocycle its pillar-like shape. In this work, 1,4-diethoxybenzene was used as the building block to synthesize pillar[5]arene. The confirmation of the pillar[5]arene was done through the use of Nuclear Resonance Spectroscopy (NMR) and the pillar[5]arene was further characterized by Infra-Red, UV-Visible, and fluorescence spectroscopy. The main focus of this research is the investigation of the host guest inclusion properties of this host with 7-methoxycoumarin (7-MC) as a fluorescent guest. Host-guest inclusion was studied in both cyclohexane and acetonitrile, to investigate the effect that polarity has on the fluorescence and binding constant of this system.
PC-G-1
Andrew Walsh
Dalhousie University

Computational Modelling of the Phosphorylation Mechanism between ATP and Glucose
Andrew Walsh\textsuperscript{a}, Arpita Yadav\textsuperscript{b}, Raymond Poirier\textsuperscript{a}

\textsuperscript{a}Memorial University of Newfoundland
\textsuperscript{b}University Institute of Engineering and Technology Chhatrapati Shahuji Maharaj University

Microbes have found ways to circumvent certain structural classes of drugs and are no longer susceptible to therapeutic drugs. Continued selective pressure by various drugs leads the way to the concept of multidrug resistance. (1) One way to solve this issue is by looking at the mechanism of phosphorylation. One antibiotic, kanamycin, is susceptible to being phosphorylated while in the body. (2) If the phosphorylation of antibiotics can be prevented, then they would be able to bind to enzymes more easily and thus allowing them to be more effective. The two-step mechanism for the phosphorylation of glucose using adenosine triphosphate (ATP), in which ATP is dephosphorylated in the first step and glucose is phosphorylated in the second step, is investigated using Hartree-Fock (HF) and B3LYP calculations. Glucose is chosen for study since it is a simple model for kanamycin. The ability of each conformer of ATP to donate a phosphate group is also presented. The phosphorylation of both the alpha and beta anomers of glucose and both the $\beta$ and $\alpha$ enantiomers of glucose is also presented.
X-ray spectroscopy study of some gold and alloy nanoclusters

David Morris and Peng Zhang*

X-ray absorption spectroscopy is a powerful technique which allows for the electronic properties and structural information to be determined for a given sample. This talk will cover how this technique can be utilized in the analysis of gold and alloy nanoclusters to obtain a better understanding of the relationship that structure and properties play. A variety of gold-based mono-metallic and bi-metallic nanoclusters will be compared to show the varying properties and structure between different types of noble metal nanoclusters. Both x-ray absorption near-edge structure (XANES) and extended x-ray absorption fine structure (EXAFS) analysis will be shown, to illustrate how these techniques compliment each other to provide a clear understanding of the relationship between properties and structures in these noble metal nanoclusters. Applications of these noble metal nanoclusters will also be briefly shown, highlighting the importance of obtaining a fundamental understanding of the structure and properties these nanoclusters possess.
PC-G-3
David Do
Dalhousie University

X-ray Absorption Spectroscopy Studies of Some Bimetallic Nano-catalysts
David Do and Peng Zhang*

Bimetallic nanoparticle catalysts often show unique properties in catalysis, and as such, it is useful to study their structural properties. X-ray absorption spectroscopy in particular is element-specific, and thus can analyze both metals that comprise a bimetallic nanoparticle. One example of a bimetallic nanoparticle catalyst to be presented in this contribution is a manganese cobalt oxide/nitrogen-doped multiwalled carbon nanotube hybrid (Mn$_x$Co$_{3-x}$O$_4$@NCNT). These nanotube hybrids showed high oxygen reduction and evolution reaction activity in electrocatalytic analysis. Through x-ray absorption near-edge spectroscopy (XANES), multiple nanotubes with varying levels of manganese and cobalt were studied and the bonding properties of the best performing catalyst were revealed. Extended x-ray absorption spectroscopy (EXAFS) analysis was used to further provide evidence as to why that particular nanotube performed better than others by looking at its local structure and properties. X-ray results on other bimetallic nanoparticles will also be presented to further the understanding of their role in catalysis.
Abstracts: Posters
IN-UP-0
Barbora Balónová
University of New Brunswick—Fredericton

Emission Modulation of Iridium Complexes via Host-Guest Chemistry
Barbora Balónová and Barry Blight*

Iridium complexes (with various N^C ligands) are undergoing intensive investigation, due to their excellent performance when used as emitters in phosphorescent organic light emitting diodes (PhOLEDs). To fulfill the requirements of full-colour OLED displays, the colour regulation (towards blue, green and red emissions) is highly desirable. In this study, we are exploring the colour tuning of different iridium emitters by host-guest assembly with DNA base-pair-like interactions in super strong hydrogen bonded arrays. The ideal interactions for holding supramolecular systems together are hydrogen bonds, as they combine relatively strong intermolecular attractions with excellent reversibility. Our findings suggest that this methodology for colour tuning can negate the synthetic manipulation of the ligand structure around iridium, which is often costly and time consuming. We are analyzing the chromaticity of iridium complexes by simply varying the concentration of compliment-guest, while examining the strength of binding and change in the emission properties. This approach focuses on supramolecular chemistry combined with synthesis, which can lead to novel materials with dynamic properties.
Femme Fatale: Understand the time required for removing an estrogen

Clarke Brown, Roderick Chisholm*

With the use of estrogenic drugs, natural production and accumulation of estrogens, there is an increased cause for concern for the environment due to estrogen having a large toxicity to many species. The no observable effect concentration has been noted to be 1 ng/L for some estrogens. This research explores the use of Chlorophytum comosum as a tool for the removal of estrogens and potentially allow for the use of vascular plants in waste water facilities. Solid phase extraction and gas chromatography mass spectrometry methods were employed to determine the concentration of the estrogens from water samples that were spiked with a known concentration of estrogens. It was found that over time the plants were able to reduce the concentration of the estrogen to below detectable limits. The results of this study encourage more work to be done and to get a more accurate model of the rate of uptake within the first several minutes, hours, and days of having a plant present.
Birch Bark-Oil (Maskwiomin): Synthesis and Analysis of an L’nu Indigenous Skin Ointment
Sarah Boudreau, Raj Kalia, David Irwin, Tuma Young, and Matthias Bierenstiel*

Maskwiomin (birch bark-oil) is an almost forgotten L’nu medicine for the topical treatment of skin conditions including psoriasis, eczema, and rashes. Bierenstiel and Young have worked with the Indigenous community of Membertou, Sydney, Nova Scotia over the past four years using a 2-Eyed Seeing approach to re-discover maskwiomin through recreation, stories, and empirical chemical research.

The L’nu method of producing the oil involves torrefaction in a campfire using a “can over can” process in which a larger can containing birch bark is exposed to heat that produces oil which can drip through a hole in the bottom to a receptacle can underneath. From a chemistry standpoint, this method has a high degree of variability as the fire conditions are difficult to reproduce. The Bierenstiel group has been developing a process to control the conditions of this process with an electrical and temperature-controlled reactor. The oil production can now be better controlled, leading to better reproducibility of series of experiments. To analyze the oil created in lab, we can use FTIR, GC-MS, GC-FID, UPLC-MS and NMR for chemical analysis. For biological analysis, we can use zone of inhibition measurement and MIC to investigate antibiotic properties.

Chemistry and microbiology studies have shown that birch bark-oil is a complex organic mixture composed of likely derivatives of betulin, a known secondary metabolite in birch bark. Betulin has antibacterial, anti-cancer, anti-viral, anti-inflammatory, and antimicrobial properties.1-3 It is a broadspectrum antibiotic against Gram+ and Gram- strains with the same efficacy as antibiotics that are available commercially.

The goals of this research project are to measure the reproducibility of obtaining birch bark-oil using the electric reactor and to modify the conditions of the reaction to obtain better results. These conditions include temperature profiles, the shape and surface of bark, the humidity and moisture of the bark, and the presence of oxygen.

Irregular changes in climate occur with increasing frequency and are a significant threat to global prosperity, threatening agricultural and biofuel industries which could lead to mass food shortages and loss of fuel production. By improving our understanding of biological phenomena such as light-adaptation in photosynthetic organisms, strategies to enhance plant-growth efficiency can be developed. Third Harmonic Generation (THG) microscopy is a novel non-invasive and bleach-free imaging technique, capable of in vivo biological interrogation. However, intrinsic THG from biological structures is limited to cell membranes and lipid droplets, hence, there is an opportunity to develop molecular labels for THG, termed harmonophores. The ability of a molecule to produce THG is determined by its second hyperpolarizability ($\gamma$) magnitude. In this study we investigate potential harmonophores quercetin dehydrate, usnic acid, β-carotene, and curcumin, in order to establish the optimal molecular structures needed for efficient harmonophores. Solutions containing different harmonophore concentrations were measured using the THG ratio technique, and with a refractometer. The $\gamma$ value of usnic acid, an inexpensive molecule found in lichens, was found to be $+0.64 \pm 0.09 \times 10^{-41} \text{m}^2/\text{V}^2$, approximately 15× larger than a similar molecule, quercetin dihydrate, indicating the polarity from additional carbonyl groups may increase THG signal. Previous research showed increased conjugation and addition of aromatic rings enhances THG. Therefore, curcumin was measured, giving a $\gamma$ value of $-1.2 \pm 0.2 \times 10^{-41} \text{m}^2/\text{V}^2$ which is the same order of magnitude as β-carotene, a previously successful harmonophore, indicating that it can be used as a label for THG microscopy.
OR-UP-1
Jacob Campbell
Saint Mary’s University

N-Demethylation of the Pseudo Opioid, Dextromethorphan Using Magnetite
Jacob Campbell and Robert Singer*

The N-Demethylation of the pseudo-opioid, dextromethorphan, has been demonstrated using a mechanochemical, modified Polonovski Reaction that utilizes magnetite as a catalyst. The methodology reported here applies a previously studied mechanochemical approach that allows for microliter quantities of liquid additives thus increasing the overall “Greenness” of the reaction. This methodology also employs the mineral magnetite, which is an iron oxide containing mineral containing both Fe(II) and Fe(III), as a catalyst. This “green” methodology has afforded comparable isolated yields of the N-demethylated product relative to previous reports from our research group.
Organic reducing agents are a class of organic molecules that readily release electrons, and are often useful alternatives to metal reductants, as they can offer milder reaction conditions and unique selectivity. In contrast to metal reductants, organic reducing agents have the advantage of facile tunability which allows for modifications to their structures to alter their redox properties. This is the case with the organic bispyridinylidene (BPY) scaffold. The BPY scaffold was modified to incorporate strongly π-donating phosphonium ylidyl groups on the backbone. Currently, this phosphonium ylidyl substituted BPY has the strongest reduction potential for a di-substituted BPY, so there is great interest in its use as a reducing agent. This poster will outline the use of this compound as a reducing agent in attempts to reduce inorganic substrates, such as chlorophosphonium salts.
AN-UP-2
Samantha Corkum and Alysson Jones
Dalhousie University

Enfamil A+™ Failing Newborn Babies? An Analysis of Carrageenan in Infant Formula
Samantha Corkum, Alysson Jones, and Roderick Chisholm*

Carrageenan is a polysaccharide derived from red seaweed which is widely used as a gelling and stabilizing agent in processed food. In recent years the safety of carrageenan in the food industry has become a topic of inquiry because the daily intake demographics and long-term effects in the human body are not widely understood.\(^1\) Kappa carrageenan was targeted as it more easily depolymerizes into the harmful low molecular weight form correlated with gastrointestinal distress in mammalian models.\(^1,2\) The goal of this study was to apply ATR-IR spectroscopy to identify the type of carrageenan in Enfamil A+® Infant Formula - Ready to Feed meal supplement for newborns. The quantification of carrageenan in the formula was performed by the barium chloride-gelatin assay. The results of this study were inconclusive due to an inability to successfully extract a carrageenan sample from the infant formula. ATR-IR spectra did not lead to the identification of the type of carrageenan present but did show expected sulfate peaks. Whether the isolated sulfate was free or bound to carrageenan was not determined. The limit of detection of the BaCl\(_2\) - gelatin assay was determined to be significantly higher than the experimental values; therefore, the results were not conclusive. Further research needs to be done in order to develop an extraction protocol for carrageenan from food samples and to create a more sensitive assay procedure.

![Structures of the repeating units of three types of carrageenan used as food additives. (Source: Food & Function 2018)](image)

Figure 1. Structures of the repeating units of three types of carrageenan used as food additives. (Source: Food & Function 2018)
Isolation of anti-mycobacterial molecules from Lentzea strains to search for new anti-tuberculosis compounds

Julie Anne Dayrit and Clarissa Sit*

Tuberculosis remains one of the top ten causes of death worldwide. Therefore, immediate discovery of new antibiotic compounds is crucial for counteracting the evolving antibiotic resistance in strains of *Mycobacterium tuberculosis* and related species. Previous studies have shown that a soil bacterium, *Lentzea kentuckyensis*, can biosynthesize lassomycin, a peptide that can kill multi-drug resistant *M. tuberculosis*. Two *Lentzea* strains were grown and observed to exhibit inhibitory activity against *M. Smegmatis*. Extracts were extracted and the active compound were isolated using column chromatography and LC/MS. Structure elucidation of the molecules by MS/MS and NMR spectroscopy is ongoing. Further studies will focus on determining the mechanism of action of the active compounds. Characterizing these metabolites will provide a better understanding of how *Lentzea* strains both interact with and defend themselves against competing microbes, such as mycobacteria.
BI-GP-1

Abdurrahman Elajmi
Saint Mary’s University

Nova Scotian Honeybees as Potential Sources for Antimicrobial Compounds against American Foulbrood Disease.

Abdurrahman Elajmi, Kooshna Prashansa, and Clarissa Sit

This study aims to figure out the gram-positive bacterium called Paenibacillus larvae causes American Foulbrood (AFB), the most serious disease of honey bees found in many countries. Several laboratory tests have been made about AFB, especially in the last 20 years. However, the creamy or dark brown, glue-like larval continues to remain the most obvious clinical symptom of AFB. There are a number of delicate and selective cultures available to isolate this spore-forming bacterium. This review will place these recent developments about the American Foulbrood. Our study involves searching for microbes that have inhibitory effects against P. larvae found in Nova Scotian honeybees. To date, more than 200 isolates have been obtained from our beehive swabs samples as well as from the bees ' external. Using pairwise assay, they are screened for P. larvae inhibition. The inhibition of microbes that restrict the growth of P. larvae is further investigated for P. larvae inhibition. Our objective is to extract and characterize secondary metabolites that cause HPLC and LC / MS inhibition.
In the continuous pursuit of effective anticancer agents, we have focused our research on curcumin analogs. A phytochemical found in the widely consumed spice turmeric, curcumin has displayed encouraging anticancer properties in clinical trials. Owing to poor pharmacokinetic profile, curcumin has not culminated into a successful anticancer drug. In an attempt to overcome these challenges, analogues of curcumin where the carbocyclic aromatic ring was replaced with heteroaromatics such as and the diarylheptanoid framework of the curcumin was retained. These compounds are expected to display interesting antioxidant properties as the mechanism of antioxidant action like curcumin while being more soluble in the aqueous medium. Double aldol condensation on appropriate β-diketones with heteroatomic-carboxaldehyde in presence of boron oxide resulted in the formation of the designed compounds. Eight compounds were successfully synthesized using conventional heating procedure. Results obtained thus far will be presented. Research supported by NSERC Discovery Grant. K.F. is supported by Jeremy Ingham Cancer Research Award from the Beatrice Hunter Cancer Research Institute. K.F. is a BSc (Chemistry, 3rd Year) student.
IN-UP-2
Tanner George
Saint Mary’s University

Mixed Donor Bidentate Ligand for Diverse Metal Chelation
Tanner George

Following prior research into a sterically bulky phosphine imine ligand (ImPPh₂), further inquiry into the group 16 element derivatives (ImPPh₂-E, E = O, S, Se, Te, A) will be explored. Current research thus far has focused on the formation of phosphine sulfide and selenide derivatives enabling potential chelation of metals between the hard imine nitrogen and the progressively softer group 16 center. Tellurium addition in the elemental state was not successful, though future efforts will be made with tellurium transfer agents since elemental tellurium was unreactive towards ImPPh₂ when heated up to 160°C in mesitylene over the course of four days. Additionally, alkylation of the phosphorus center with 9-bromofluorene gave the fluorenyl derivative (ImPPh₂-FluBr). This ligand, in the anionic form, has the potential to chelate to metals via σ-donation from the imine, and either 2-electron σ-donation (ylide form, B) or 6-electron π-donation from the fluorenyl group (C).
MA-UP-1
Elvin Girineza
St. Francis Xavier University

Application of Cu(I) Oxide/Semiconductor Hybrids in Light-Driven Click Chemistry
Elvin Girineza, Dreenan A. Shea, and Geniece Hallett-Tapley*

Click chemistry is one of the most widely employed two-step coupling mechanisms with applications in biosciences, drug discovery and material science. The most widely recognized coupling mechanism is the Huisgen 1,3-dipolar cycloaddition of azides and terminal alkynes. The discovery by Sharpless and coworkers implementing Cu(I) catalysts to improve upon the efficiency of this coupling reaction was an experimental breakthrough that has led to the development of compounds with wide reaching applications in clinical chemotherapy for both antiviral and anticancer treatments.¹ However, many of the pathways implemented, to date, still suffer from lengthy reaction times and elevated reaction temperatures. Moreover, the traditional pathway relies on the use of homogenous Cu (I) sources, limiting sustainability of this cycloaddition. Given the emergence of green chemistry initiatives, marling the characteristics of Cu (I) into potentially recyclable, heterogeneous materials and using more sustainable energy sources to drive the reaction, such as a photocatalytic approach,² is of considerable interest.

Cu₂O is a potential alternative to traditional homogenous, Cu (I) sources due to its small band-gap and visible light-activation. The current contribution will examine the synthesis of a series of Cu₂O/semiconductor hybrids (TiO₂, KNbO₃) for applications in light-activated cycloaddition of benzyl azide and phenylacetylene to form 1,2,3-triazole rings. Preliminary results will discuss the influence of irradiation source, substrate and catalyst concentration, as well as reaction time on the overall efficiency of Cu₂O-mediated photocatalytic click chemistry.

Ionic thiourea catalysis have a wide range of potential applications including use as recyclable organocatalysts. Organocatalysis is valuable due to the reduced cost and environmental impact of organocatalysts compared to metal catalysts and the fact that organocatalysts can be tailored for a specific reaction. Our research involves the synthesis of a range of ionic thiourea based compounds using a modular approach and has previously shown that ionic thiourea based compounds are effective co-catalysts for the Morita-Bayliss-Hillman reaction. The next phase of research will involve studying a bis-thiourea compound for catalytic activity in the Morita-Bayliss-Hillman reaction and testing several other thiourea compounds for catalytic activity in Friedel-Crafts acylations and Diels-Alder reactions. Recent advances and proposed directions for this research will be discussed.

Reactivity of (PSiP)M(H)(NHR) (M = Rh, Ir; R = aryl, alkyl, H) Complexes with Unsaturated Substrates: Investigating Insertion into the M-N bond

Helia Hollenhorst, Erin Morgan, and Laura Turculet*

The N-H bond oxidative addition of ammonia and anilines by bis(phosphino)silyl (Cy-PSiP)Ir (Cy-PSiP = κ³-(2-Cy₂PC₆H₄)₂SiMe) pincer complexes has previously been reported by the Turculet group. Given the prevalence of nitrogen containing compounds in many pharmaceuticals and fine chemicals, we sought to explore the reactivity of amido and anilido complexes prepared by such oxidative addition processes, with the goal of developing new reactivity applicable to the functionalization of amines. In this regard, we have investigated the reactivity of Rh and Ir amido hydride complexes supported by silyl pincer ligation towards various unsaturated substrates, in an effort to explore the potential for insertion into the metal-amido bond. Our efforts in this regard will be detailed in this presentation.
AN-UP-3
Toren Hynes
Dalhousie University

Optimising 3-phenyl-1,4,2-dioxazol-5-one as an Electrolyte Additive for Lithium-Ion Cells
Toren Hynes, David Hall, and Jeff Dahn*

An effective method to reduce carbon dioxide emissions is to switch to renewables for energy generation and transportation. Since current sources of renewable energy, such as wind and solar, are intermittent, it is essential to find ways to store energy to match supply and demand. If vehicles are to be powered by renewable energy, they need portable energy storage. Currently, lithium-ion batteries are one of the most viable solutions for energy storage. Extending the lifespan of lithium-ion batteries is the goal of this research, carried out with Dr. David Hall of Dr. Jeff Dahn’s research group at Dalhousie University in late 2017. We developed and tested a chemical compound, 3-phenyl-1,4,2-dioxazol-5-one (PDO), which greatly improves the lifespan of lithium-ion batteries. One percent of this by weight in a cell’s electrolyte, along with two percent ethylene sulfate, will extend a battery’s lifespan more than three-fold over conventional vinylene carbonate-containing electrolyte.
IN-UP-3
Dakshita Jagota
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Synthesis and study of iron coordination complexes for catalytic reactions of carbon dioxide with epoxides

Dakshita Jagota, Kori Andrea, and Francesca Kerton*

Production of cyclic carbonates from the reactions of carbon dioxide (CO$_2$) and epoxides is important as it utilizes CO$_2$ as a renewable and inexpensive C-1 source. These products have a wide range of applications such as fillers in cosmetics, polar aprotic solvents for synthesis and electrochemical applications and reagents in polycarbonate formation. Industrially, the conversion of CO$_2$ and epoxides to cyclic carbonates typically requires very harsh conditions such as high pressures and temperatures; however, much research has taken place to allow this transformation to occur under milder conditions with the use of a catalyst.$^1$ The Kerton group focuses on iron based catalytic systems due to iron’s high abundance in the Earth’s crust, low toxicity, and cost-effectiveness. Iron amino-bis(phenolate) compounds including chlorido and µ-oxo derivatives were synthesized to be used as catalysts in these transformations. In the presence of a cocatalyst under solvent-free conditions, the oxo-complexes demonstrated poor reactivity for the reaction of CO$_2$ and epoxides. We were intrigued by an interesting colour change from purple to red when the monometallic iron chloride species were used in coupling reactions. We found this was due to an epoxide deoxygenation of the substrate leading to the formation of the corresponding iron(III) µ-oxo compounds which can then enter their own catalytic cycle.$^2$ Deoxygenation of epoxides when using catalysts for the production of cyclic carbonates is a process that has been overlooked by chemists. This reaction may lead to catalyst deactivation and thus formation of such compounds needs to be prevented in future catalyst design.

MA-UP-2
Nikita Kenney
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Nickel/Potassium Niobium Oxides as Photocatalysts for C-C Coupling
Nikita Kenney and Geniece L. Hallet-Tapley*

There has been an increasing emphasis on the development of environmentally sustainable and benign chemical routes among researchers and in industry. C-C bond formation, although crucial to organic synthesis, requires elevated temperatures and prolonged reaction times to promote. The Heck reaction, important in the synthesis of compounds such as Naproxen™ and Singulair™, presents considerable potential for optimization to a more sustainable process. Traditional methods of promoting the Heck reaction rely on elevated temperatures, prolonged reaction times (8-72 hours), use of costly Pd derived materials and environmentally undesirable solvents.¹ In an effort to reduce the overall energy consumption and economic impact of the Heck reaction, the current contribution will examine the design and synthesis of retrievable and light-activated NiO nanoparticle/niobium oxide perovskite composites for use as potential alternative C-C coupling catalysts. C-C coupling between styrene and iodobenzene will be used as the initial screening reaction. The aforementioned reaction will be examined in the absence of external heating, relying on excitation of the photocatalyst with blue, 455 nm LED light and the resultant localized surface plasmon resonance effect to promote the reaction. A variety of experimental parameters will be discussed, including solvent effects, base effects, light intensity, and reaction time.

MA-UP-3
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Mount Allison University

Assessment of Non-monotonic trends in Nanoparticle Film Hydrophobicity by variation of Ligand Shell Composition
Annabelle Kilham, Rachel Howlett, M.-Vicki Meli*

Nanoscale wetting is an important area of research due to its many biological and technological applications. The hydrophobicity of films formed from five nanometer core gold nanoparticles capped with varying mixtures of methyl and hydroxyl groups was tested using contact angle analysis. The mixtures investigated consisted of 2%-hydroxyl terminated, 25%-hydroxyl terminated, and 50%-hydroxyl terminated nanoparticles as well as a 100%-methyl terminated group. The films were formed on a silicon substrate via spin-coating and subsequent dropwise deposition to ensure complete coverage. The contact angle measurements using deionized water were taken directly after film formation with a goniometer and the coverage of the films was evaluated with atomic force microscopy. The contact angle results revealed non-monotonic wetting trends with an increase in the hydrophobicity of films composed of the 2%-hydroxyl terminated and the 25%-hydroxyl terminated nanoparticles. Investigating the unusual trend in the hydrophobicity of nanoparticle films due to ligand shell composition will lead to greater understanding of the films and control over their properties.
IN-GP-2
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Synthesis of a “redox-confused” Bi(I/III) tri-amide
Marcus Kindervater, Katherine Marczenko*, and Saurabh Chitnis*

Low-oxidation state main group compounds are of significant interest as models for bonding theory and stoichiometric or catalytic activation of challenging bonds. These species have traditionally been synthesized by reduction of higher oxidation state element halides using external reductants. However, alternatives such as the use of redox-active ligands have since gained interest as electron acceptors not requiring the use of sacrificial reducing agents. Herein, we report the synthesis and characterization of a 10-electron 3-coordinate bismuth tri-amide with a planar T-shape ground state geometry. This system was characterized by solution and solid state NMR, X-ray crystallography, UV-VIS spectroscopy and supported by dispersion-corrected DFT calculations. Molecular and electronic structure of this tethered tri-amide ligated bismuth complex suggest significant Bi(I) character but was found to behave like a traditional Bi(III) source. This “redox-confused” Bi(I/III) behavior bodes well for exploring an ill-defined redox couple in the p-block.
Estimates of the thermodynamic parameters of micellization (ΔmicG°, ΔmicH°, and ΔmicS°) have been determined for a series of mixed micelles consisting of ionic surfactants (sodium dodecylsulfate and dodecyltrimethylammonium bromide) and medium chain length alcohols as the co surfactant. The enthalpies of micellization have been measured directly for the above systems using isoperibol solution calorimetry; the Gibbs energies and entropies of micellization are obtained by application of the mass-action model to the critical micelle concentration values from the calorimetric titration experiments. The thermodynamic properties of mixed micelle formation with alcohol concentration and temperature are in excellent agreement with our previous results. However, there does appear to be some dependence of the thermodynamic properties of mixed micelle formation on the chain length of the alcohol. These dependencies are discussed in terms of the manner in which the alcohol interacts with the ionic head groups and the location of the solubilizates in the micellar interior.
Contamination of the global water ways by industrial waste is a pressing environmental issue and global availability of clean drinking water remains a struggle. Many common drugs, including 17b-estradiol, are present in water samples and have been proven to bioaccumulate within human tissues. To date, research in this area has been focused on the use of light as of means of “photodegrading” these aqueous pollutants using high energy UV light sources that are non-selective and damaging to other inhabitants of the water ecosystem. The use of light-activated solids with visible light response may improve upon this process.

Previous work in our group has demonstrated the photocatalytic diversity of niobium oxides. Moreover, potassium niobium oxide (KNbO₃), a solid with similar light-active properties to TiO₂, holds a clear advantage due to its larger particle size (~1 mm), allowing for more facile catalyst recovery and reuse – a characteristic in high demand given the global shift towards green chemistry initiatives. Decoration of the KNbO₃ surface with Au nanospheres (AuNP; λ_max = 530 nm) can increase the response of the solid to favour the use of lower energy, visible light via surface plasmon resonance of the nanoparticle surface. The research to be discussed will examine the ability of visible light activated AuNP/KNbO₃ to facilitate estradiol. The influence of photocatalyst and pollutant concentrations, as well as irradiation time will be investigated.

Excited State Intramolecular Proton Transfer Reactions in Polyaryl Bisphenols

Jenna McNutt and Matthew Lukeman*

Electronic excitation of phenols can produce a significant increase in acidity, causing the phenolic proton to transfer to basic sites on the same molecule in a reaction called an excited state intramolecular proton transfer (ESIPT). This work involves the investigation of the photochemistry of polyaryls containing two hydroxyl groups.

1,4-di(o-hydroxyphenyl)naphthalene (7) and 2-phenylresorcinol (9) were prepared using a methodology involving Suzuki coupling and demethylation, and were obtained in crude yields of 65% and 59%, respectively. Photochemical studies, including UV-Vis spectroscopy, product studies, and fluorescence spectroscopy, were performed on bisphenols p-di(o-hydroxyphenyl)benzene (6), 7, and 9. Phenol 6 underwent ESIPT and reverse proton transfer (RPT) inefficiently (Φ < 0.01), as indicated by deuterium incorporation on the central aromatic ring. In addition, a competing side reaction was observed which gave unidentified products. ESIPT and electrocyclic ring closure (ERC) took place on irradiation of 7, and the reaction proceeded cleanly with no side products. The cyclized photoproduct appeared to undergo aromatization on exposure to air. Phenol 9 underwent ESIPT and RPT which gave efficient deuterium incorporation (Φ = 0.25) at the 2'-position.

The results suggest that placement of two electron-donating phenolic hydroxyl groups on the same ‘donor’ ring leads to an enhancement of ESIPT reaction efficiency, whereas placement of these two hydroxyl groups opposite to one another on different rings leads to reduced ESIPT efficiency. This is consistent with a reaction mechanism that involves substantial excited state charge transfer prior to the proton transfer step.
Fluorescence Based Investigations of Photophysical Properties of 4,5-didecoxypyrene Oligomers in Cyclohexane Solution

Tara Misener and Brian Wagner*

Photophysical properties of the cyclohexane solubilized monomer-through-pentamer series of oligomers of 4,5-didecoxypyrene (synthesized by the Bodwell Group at Memorial University) were investigated via fluorescence spectroscopy. Quantum yield and time-resolved lifetime experiments were conducted, which allowed for the determination of radiative and nonradiative rate constants. Trends in emission spectra maxima demonstrated that the oligomers were red-shifted relative to the monomer due to elongation and increased delocalization of the electrons. Quantum yield increased from the monomer to the dimer, but levelled off at 0.80 for the trimer, tetramer and pentamer. Lifetime decreased from the monomer and levelled off at the tetramer. In addition to this, the radiative and nonradiative rate constants both increased from the monomer. However, the radiative rate constant increased more than the nonradiative rate constant did, resulting in the increased quantum yield of the larger compounds. Furthermore, an increase in radiative and nonradiative rate constants results in a faster rate at which an excited molecule decays, thereby decreasing the lifetime of the compounds. The trimer, tetramer and pentamer compounds exist in the liquid state at room temperature and are intensely fluorescent as both neat liquid and in dilute solution. Therefore, they are considered to be functional molecular liquids (FML), with a number of potential applications.
Neutralization of Paper Pulp Waste Associated with Bottle Recycling
Soraya Moore, Christina Bottaro, and Kelly Hawboldt

Ever Green Recycling is a non-profit organization that provides meaningful and sustainable employment for individuals with moderate to severe mental illness while also providing green solutions to waste management in Newfoundland and Labrador. Ever Green seeks out opportunities to maximize resource recovery in local businesses, and one area they have identified is pulp generated in label removal in the beverage industry. The bottle recycling process is designed for the complete re-use of bottles which requires the removal of bottle labels. However, the treatment solvent of NaOH in water used to remove the labels increases the pH of the recovered paper pulp to very highly basic pH (>10) and this high basicity represents as a safety issue for the workers handling the pulp. To address this issue, the pH and other bulk properties of the pulp will be examined, literature for methods to remove or reduce the NaOH content of the pulp will be reviewed, and the most promising processes (e.g. filter press) will be tested while the properties of the pulp before and after treatment are monitored. The outcome of this project will be recommendations on the feasibility of removing the NaOH and water, and possible treatment options.
Mechanistic Studies of Excitation Energy Transfer in Photosynthetic Light-Harvesting Complexes
Katherine Parsons and Aaron Kelly*

The photosynthetic apparatus in higher plants responsible for harnessing the sun’s energy for photosynthesis can be considered to consist of two essential components; (i) the peripheral antennae and (ii) the reaction center. In order for the later steps of photosynthesis to proceed the peripheral antennae must harvest and transfer the sun’s energy to the reaction center. The peripheral antennae are light-harvesting complexes, such as the light-harvesting complex II (LHClI) and the minor complex Chlorophyll Protein 26 (CP26). These light-harvesting complexes are composed of multiple pigment molecules that are bound by a protein matrix. When a pigment molecule absorbs a photon, an electronic excitation occurs in that molecule, which is then eventually transferred to the reaction center. In this work, the pathways in which electronic excitation energy travels through individual LHClI and CP26 complexes are studied by utilizing quantum-classical dynamics simulations. The effect of temperature on the mechanism, as well as the effect of the initial location of the excitation, are examined. Further research will extend to multiple complexes to help develop a more complete mechanistic picture of the light-harvesting process.
Dissolved organic matter (DOM) is one of the most significant sources of carbon in aquatic environments and can be found in all water sources. This reservoir of reduced carbon plays an active role in the carbon cycle. Due to the chemical complexity of DOM, exactly how it participates in the carbon cycle is difficult to determine. On a fundamental level, the functional groups present in the DOM will to some extent control the behaviour of DOM in aquatic environments. Here we present a preliminary study comparing the utility of infrared and raman spectroscopy for characterizing the functional group nature of DOM. Water samples were taken at two locations, upstream Savage Creek, NL (SC, freshwater) and Outer Cove Beach, NL (OCB), where Savage Creek meets the Atlantic Ocean. DOM was isolated using solid phase extraction, and extracts were analyzed with IR and Raman. This allowed for the determination of the functional groups which were present in the isolated DOM, and what changes occur in the freshwater-marine mixing zone. The analyses allow for an approximation of relative concentration of each functional group across samples. The comparison between IR and Raman spectra present a potentially new avenue for DOM analysis. By further characterization of DOM within water samples, we can better understand the ecological effects of DOM and its various roles within the carbon cycle.
AN-UP-6
Morrigan Payne and Harrison Max
Dalhousie University

Quantifying Lead and Aluminum Ion Concentrations in Recreational Cannabis
Morrigan Payne, Harrison Max, and Roderick Chisholm*

Due to its long-time status as an illicit substance, research of issues in the cannabis industry has been extremely limited. Cannabis has been well characterized as a hyperaccumulator of heavy metals, however Health Canada has not defined a concentration limit for these potentially harmful metal ions. The goal of this experiment was to use an acid-digested recreational cannabis sample and test for Pb$^{2+}$ and Al$^{3+}$ ions using atomic absorption spectroscopy and titration methods. Pb$^{2+}$ was found to be at a concentration of 18.0 ± 0.2 mg/kg cannabis, while Al$^{3+}$ was found to be at 2714 mg/kg cannabis.
MA-UP-6
Rahul Pongasseril Lal
Cape Breton University

Electrical applications of bio-char from forestry residue
Rahul Pongasseril Lal and Stephanie MacQuarrie*

Carbon is used for a wide variety of applications in the field of electrical engineering; one of the latest trends in this field is the utilization of carbon in energy storage applications. Among carbon capacitors, about 60% of the cost is due to carbon. Raw biochar has been considered as a potential means of storing significant carbon for long periods to mitigate green house gas emissions. A number of studies conducted using biochar as a supercapacitor material suggests that it is a good source of energy storage. This work focuses on determining the conductivity of various chars generated from forestry residues and subjected to oxidation processes. The study conducted on the forestry biochar suggests that char shows a conductivity varying from 25 to 50 siemens per meter based on the applied force varying from 1000 lbs to 5000 lbs. The char was oxidised using modified Hummers method and further testing under the same condition showed that the conductivity was greatly reduced.
AN-UP-7
Katherine Purvis
Saint Mary’s University

Determination of the Origin of Third Harmonic Generation from Cyanobacteria
Katherine Purvis, Kennedy Brittain, Ariana Joseph, Richard Cisek, and Danielle Tokarz*

The role of phycobiliproteins in the origin of third harmonic generation (THG) signal from cyanobacteria was investigated to characterize the THG for potential use in imaging and analysis of cyanobacteria, to improve our understanding of photosynthesis, and to determine if phycobiliproteins can be used as dyes for in vivo THG microscopy. The second hyperpolarizability ($\gamma$) values for key phycobiliproteins within cyanobacteria: CL-allophycocyanin, R-phycoerythrin and C-phycocyanin, were measured using the THG ratio technique, combined with index of refraction measurements, to determine the strength of the THG signal from a phycobiliprotein molecule. The $\gamma$ of phycocyanobilin, a phycobilin that is found within CL-allophycocyanin and C-phycocyanin, was also measured to establish the origin of the THG signal from within individual phycobiliproteins. The experimentally determined high $\gamma$ values of the phycobiliprotein indicate that they are one of the primary contributors to the THG generated from cyanobacteria. Furthermore, it was found that the estimated $\gamma$ values of the phycobiliproteins using the phycocyanobilin $\gamma$ value were within experimental uncertainty of the measured $\gamma$ values of the phycobiliproteins, indicating that this phycobilin is the primary molecule within phycobiliproteins generating the THG signal. When compared to $\gamma$ of a standard THG label, $\beta$-carotene, phycocyanobilin’s $\gamma$ was found to be $\sim7 \times$ higher and the phycobiliproteins were found to be $\sim59-326 \times$ higher. These findings indicate that phycobiliproteins and phycobilins could be used as novel water-soluble and nontoxic dyes for THG microscopy.
On October 17, 2018, in Canada, Cannabis was legalized for recreational use. There are 149 different licensed retailers are used to quantify the cannabinoids within the Cannabis plant and grow the plants for government issued cannabis. Therefore, due to having multiple licensed retailers all using their own methods for the quantification, there lacks a source of verification and repeatability for the process of quantifying the cannabinoids within the plant. This project focuses on the cannabinoid, THC, and how to quantify it using five different extraction methods and using GCMS as the detection. The extraction method that gives the highest THC extracted will be focused in on to see if it can be repeated and to verify that the amount of THC present in government issued Cannabis is correct. The purpose of this experiment is to determine if THC can be quantified in a repeatable, verified way.
AN-UP-9
Gaius St. Marie
Saint Mary’s University

Fabrication of Multidimensional Surface-Enhanced Raman Spectroscopy (SERS) Substrates using Bioscaffolds
Gaius St. Marie and Christa Brosseau*

Plasmonics is the field of research which explores the unique optical and electronic effects observed when certain nanoscale metals interact with light. Unfortunately, plasmonic structures are difficult and costly to prepare, which limits their widespread application in society. Therefore, there is great interest in sustainable plasmonic architectures that can be manufactured using natural materials. In this work, buttercup petals are used as bioscaffolds for the production of highly functional plasmonic materials. Scanning Electron Microscopy (SEM) and Surface-Enhanced Raman Spectroscopy (SERS) were used to characterize these buttercup petals. The SERS performance of the buttercup petal was evaluated using a strong Raman reporter para-aminothiophenol (pATP) with a focus on developing an optimal SERS substrate by varying the deposition parameters of physical vapour deposition (PVD).
With current drug use rates, as well as the recent legalization of marijuana, methods for drug usage screening (such as analysis of hair) have been employed in order to keep workplaces and other environments free from illicit drugs. Due to these tests becoming common practice, drug users have suggested methods for removing THC, from their hair, to avoid detection. This research explores these inventive methods of removing THC from one’s hair by modeling a marijuana user’s hair, and applying two of these methods to remove spiked THC. Detection of the trace THC is obtained using GC-MS. The results from this work indicate that despite the inventive methods suggested to avoid THC detection in hair, trace THC could reliably be detected in all of these methods.
Turn Down the Heat! Modified Magnesiothermic Reduction to Produce High-Surface Area Mesoporous Silicon Nanoparticles

Emily Traver, Yiqi Lai, Sarah Martell, Judy MacInnis, Stephanie MacQuarrie, and Mita Dasog*

Mesoporous silicon (mp-Si) has been extensively explored as an interesting optical material, drug delivery vehicle, sensor, gas storage medium, anode material for Li-ion batteries, and in other energy conversion systems [1]. The utility of mp-Si is highly dependent on the surface area, crystallinity, morphology, and pore volume, which are often dictated by the synthetic methods used to prepare them. Metallothermic reduction has gained significant attention as it allows for straightforward synthesis of porous Si from inexpensive precursors such as glass, sand, or sol-gel polymers. Additionally, it allows for morphology retention and can be scaled up. Magnesiothermic reduction reactions are performed at different temperatures, for varying lengths of time using different grain sizes of the metal which can negatively impact the physical properties of mp-Si [2]. This presentation will highlight a modified two-step magnesiothermic reduction process for the synthesis of mp-Si that minimizes the heat damage in traditional metallothermic reduction. This modified process enables synthesis of highest surface area mp-Si reported to date for magnesiothermic reduction.

First-Principles Prediction of the CO2 Phase Diagram
Joseph Weatherby, Alberto Otero-de-la-Roza, and Erin Johnson*

A central idea in physical chemistry is the phase diagram of a compound, which represents its thermodynamically stable states as a function of pressure and temperature. The use of dispersion-corrected density-functional theory allows for accurate calculation of the relative energies of various crystal phases. However, first-principles prediction of a solid phase diagram further requires inclusion of thermal vibrational effects within the quasi-harmonic approximation, which is extremely expensive computationally. In this work, we consider the phase diagram of carbon dioxide (CO$_2$), which is an excellent test case for theory due to its small molecular size, and the existence of controversy in the literature concerning the structure of several of its phases. Using the B86bPBE density functional, along with the exchange-hole dipole moment (XDM) dispersion correction, we aim to resolve this controversy through computational prediction of the CO$_2$ phase diagram.
A cost-effective, portable, and non-invasive approach for quantitative measurement of neonatal pulmonary edema and infection is presented. Edema and infection were determined using reflectance spectra in the near-infrared (NIR) from an 18-wavelength sensor with a light source in the NIR region. A cellulose sponge tissue phantom and a scale from an adult lung were used to model the neonatal lung. Since water is the most abundant molecule in edema, the concentration of water was changed to observe any trends. Measures were taken between 80-100% saturation. True edema was measured by weighing the tissue phantom and weighing - by difference - the amount of water added to the lung. The experiment was also performed using 3.25% milk as a model for infection. A stepwise multilinear regression was performed using MatLab (custom script). For edema, results showed that the correlating wavelengths were 410nm, 760nm, and 810nm with a standard estimating error (SEE) of 3.82%. Furthermore, for infection, the results indicate significant wavelengths are 610nm, 680nm, and 940nm with a SEE of 5.38%. A logistic regression was performed using the same datasets presented and tested whether NIR spectroscopy could be used to distinguish between edema and infection. It indicated that significant wavelengths were 610, 810, and 860nm. The results from this experiment indicate that NIR spectroscopy can differentiate between edema and infection. Overall, the results demonstrated that NIR spectroscopy can provide a new tool for clinical assessment for pulmonary edema and infection in neonates.
IN-UP-4
Craig Weir
Memorial University of Newfoundland

Getting Mixed-up: Abnormal surface area results in mixed linkers UiO-66-NH2
Craig Weir, Mason C. Lawrence and Michael J. Katz*

Metal-organic frameworks (MOFs) are a fascinating field of chemistry for their multi-use applications that is caused by their high porosity. MOFs are comprised of two main structures. The first component is the cation (also known as a node) containing a single transition metal, a pair of transition metals, or even a cluster of transition metals. The second component is an anionic organic ligand (also known as a linker).

UiO-66 is a Zr-node-containing MOF with 1,4-benzenedicarboxylate as the linker. When the dicarboxylate linker contains an amine on the phenyl ring, UiO-66-NH2 is formed. However, when a mixture of the two linkers is used, then a mixed linker MOF is formed showing a surprising result when the surface area of the mixed linker MOF is examined.

While analyzing different percent substitution of these amine ligands, an increase of surface area was observed. We hypothesize that this is due to the formation of defects in the structure of the MOF. With regards to MOFs, a defect occurs when a linker or node are missing. In this case, the data suggests that linker defects are present. The presence of fewer linkers increases the accessible surface area per gram of the material.

To better understand the source of the defects, we have been examining how the synthesis and work up of the mixed linker MOF affects the overall surface area. The following poster will present the results and findings from these analyses as well as NMR data to understand how the different linkers are affecting the defect concentration.
IN-UP-5
Jennifer Wright and Bailey Mosher
Saint Mary’s University

The Synthesis and Characterization of Bulky m-Terphenyl Cyclopentadienyl Ligands

Jennifer Wright, Bailey Mosher, Alex Veinot, and Jason D. Masuda*

Sterically hindered cyclopentadienyl (Cp) ligands are of interest due to their ability to stabilize metal centres. This allows for the isolation of molecules with unusual bonding patterns and reactivity. Over the last few years we have been interested in cyclopentadienyl ligands substituted with sterically encumbered m-terphenyl ligand substituents. These ligands are of particular interest because the aryl groups of the terphenyl can chelate through aryl-π interactions with the metal center.

A new synthetic route to bulky, more tunable, and chelating cyclopentadienyl ligands featuring m-terphenyl substituents was developed, and several alkali metal complexes were prepared and characterised both structurally and spectroscopically.\(^1\) Using structural information obtained from single crystal X-ray diffraction data, it was determined that significant interactions between the flanking aryl groups of the m-terphenyl and the metal centres do happen in some cases. Recently, we have prepared three metallocenes, \((m\text{-termesCp})_2M\) (M=Fe, Co, Ni) their corresponding metallocenium salts. These compounds have been characterized by X-ray crystallography, IR spectrometry, UV-Vis, NMR, melting point and cyclic voltammetry.

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