



Physical & Environmental Sciences
UNIVERSITY OF TORONTO
SCARBOROUGH

DIRECTED RESEARCH IN CHEMISTRY

CHMD90/91

RESEARCH PROJECTS BOOKLET

2021 Fall – 2022 Winter

CHMD90Y3 & CHMD91H3
DIRECTED RESEARCH IN CHEMISTRY

Course Coordinator: Prof. Xiao-an Zhang (xiaoan.zhang@utoronto.ca)

Admittance requirements:

- A Cumulative Grade Point Average of at least **2.3**. Students who do not meet this requirement are encouraged to enroll in [CHMD92H3](#) instead.
- Completion of at least 15 full credits
- Completion of at least 1.0 full credits of C-level CHM courses containing a lab component (i.e. CHMC16H3, CHMC31Y3, CHMC41H3 or CHMC42H3, CHMC47H3, BIOC23H3)

Plan of action for students planning to register in [CHMD90Y3](#) or [CHMD91H3](#)

1. Look through the projects listed below.
2. **Find a research supervisor** who will take you to do a project of your choice (to expedite the process send to your prospective supervisor your unofficial transcript, your CV along with the letter of intent).

Considering the restricted lab access due to Covid-19, please communicate with potential supervisor regarding the timeline. Some projects without “wet-lab” component may not be impacted by the restriction, but other project may have to be extended to the following semester, depending on when the lab can be fully accessible.

3. Request the course on ACORN and contact the course Coordinator (listed in the timetable as the instructor) to inform of your intent to take the course. Your status will be INT. You will not be officially enrolled until you complete the remaining steps (below)
4. Obtain the D90/91 Supervised Study form, which is available online at <https://www.utoronto.ca/registrar/supervised-study-form> or at the Office of the Registrar (Highland Hall, Main Floor).
5. Meet with your Supervisor and obtain their signature on a 'Supervised Study form'. Make sure the course code, supervisor name, title of the project are **clearly** printed on the form as this information will appear on your transcript. Your supervisor will also complete information regarding the grading structure of the project.
6. Collect the two required signatures under the Physical and Environmental Sciences section. The Department Chair or the Associate Chair Undergraduate can sign under the 'Chair' section; the course coordinator, Prof. Xiao-an Zhang (xiaoan.zhang@utoronto.ca) or Chemistry Discipline Representative Dr. Effie Sauer (effie.sauer@utoronto.ca) can sign under the 'Secretary' section.
7. Once the above steps are complete, please submit the form to the Assistant to the Chair (Room EV241). The completed forms will be collected and forwarded to the Registrar's Office to process enrolment. Once finalized, your course status on ACORN from interim (INT) to approved (APP). Students are advised to complete this process early so that the required forms can be submitted and processed by the last day to add courses for the session.

Note, it will be impossible to enroll without finding the research supervisor, thus this search is crucial. You could diversify your search by initiate conversations with more than one faculty members offering projects.

Course description:

These courses involve participation in an original research project under the direction of a faculty supervisor. Approximately 260 hours of work are expected in [CHMD90Y3](#) and 130 hours in [CHMD91H3](#). Topics will be selected in conference with the course coordinator who will provide project descriptions from potential faculty supervisors. Progress will be monitored through periodic consultation with the faculty supervisor as well as the submission of written reports. The final results of the project will be presented in a written thesis as well as an oral, poster or online presentation (TBD) at the end of the term.

Prerequisite: Permission of a course coordinator.

Exclusion: Students may take either [CHMD90Y3](#) or [CHMD91H3](#) but not both. Note that [CHMD92H3](#) is an exclusion to both [CHMD90Y3](#) and [CHMD91H3](#).

EVALUATION FOR CHMD90 and CHMD91:

Grade contribution:

Thesis report: 80% (Supervisor: 30%; reader A: 25%; reader B: 25%)

Presentation: 20% (presentation will be assessed by two or more evaluators, not including your supervisor/co-supervisor. Each evaluation will be weighted equally).

Important Dates for [CHMD91-Fall](#)

- **Submission deadline for the 1st draft of your thesis to your supervisor: November 26, 2021.** Find two external readers and presentation evaluators among faculty or postdoctoral fellows.
- **Final report is due December 03, 2021.**
- **Final oral, poster or online (TBD) presentation 20%** (Tentative date: December 07, 2021)
- **All marks due December 10, 2021**

Important Dates for [CHMD90](#) and [CHMD91-Winter](#)

- **Submission deadline for the 1st draft of your thesis to your supervisor: April 01, 2022.** Find two external readers presentation evaluators among faculty or postdoctoral fellows.
- **Final report is due April 08, 2022.**
- **Final oral, poster or online (TBD) presentation 20%** (Tentative date: April 12, 2022)
- **All marks due April 15, 2022**

Guidelines regarding the thesis reports: The thesis reports should be prepared in max. 20 pages, single-spaced using Times New Roman font-12 including the following sections:

1. **Title page** with the title of your project, your name and number, your supervisor(s) name, the course code, and the date of submission. **(1-page)**
2. **Table of Contents (1-page)**
3. **Abbreviations (if necessary, 1-page)**
4. **Introduction (max. 3 pages)**
5. **Experimental** with subsections such as reagents and chemicals, instruments, and procedure.
6. **Results and Discussion**
7. **Conclusions**
8. **Acknowledgments**
9. **References (max. 2 pages)** References should be prepared using the *Journal of American Chemical Society* guidelines.

Appendix can be attached to your thesis report with unlimited page numbers displaying raw experimental results such as MS, NMR, and IR data.

Lab Safety & Onboarding Training Requirements

The Department of Physical and Environmental Sciences has recently introduced new safety and on-boarding training requirements, for all new laboratory personnel, including CHMD90/91 students whose research projects include “wet-lab” components:

<https://www.utoronto.ca/physsci/onboarding-and-training>

Please carefully review the webpage. It covers guidelines for both safety training and registration requirements to gain access to the research building.

Safety Training: The EHS courses listed in the webpage above are required for wet-lab experiments. Please discuss this with your supervisor. Students are recommended to complete the online training courses on time, so there will be no delay to gain the access to the lab. Specific instructions also could be found in the Department Personnel Registration and Emergency Preparedness (PREP) document:

https://www.utoronto.ca/physsci/sites/utoronto.ca.physsci/files/u35/PREP%20Form%20Final_1.pdf

You can enroll into the required online EHS courses, including the WHMIS training via the link: <https://ehs.utoronto.ca/training/my-ehs-training/>

Training certification submission: After finishing the online training successfully, you should give/email a copy of your certificate to your supervisor.

Biosafety course: Please, consult with your supervisor whether a Biosafety Certificate is required for your project. The course can be found from the following link:

<https://ehs.utoronto.ca/our-services/biosafety/biosafety-training/>

(You should give a copy of your certificate to your supervisor)

***Note: Please, consult your supervisor about the attached NSERC Consent Form on the next page.**



Consent to Provide Limited Personal Information About Highly Qualified Personnel (HQP) to NSERC

NSERC applicants are required to describe their contributions to the training or supervision of highly qualified personnel (HQP) by providing certain details about the individuals they have trained or supervised during the six years prior to their current application. HQP information must be entered on the Personal Data Form (Form 100). This information includes the trainee's name, type of HQP training (e.g., undergraduate, master's, technical etc.) and status (completed, in-progress, incomplete), years supervised or co-supervised, title of the project or thesis, and the individual's present position.

Based on the federal *Privacy Act* rules governing the collection of personal information, applicants are asked to obtain consent from the individuals they have supervised before providing personal data about them to NSERC. In seeking this consent, the NSERC applicant must inform these individuals what data will be supplied, and assure them that it will only be used by NSERC for the purpose of assessing the applicant's contribution to HQP training. To reduce seeking consent for multiple applications, applicants will only need to seek consent one time for a six-year period. If the trainee provides consent by e-mail, the response must include confirmation that they have read and agree to the text of the consent form.

When consent cannot be obtained, applicants are asked to not provide names, or other combinations of data, that would identify those supervised. However, they may still provide the type of HQP training and status, years supervised or co-supervised, a general description of the project or thesis, and a general indication of the individual's present position if known.

An example of entering HQP information on Form 100 (with and without consent):

Name	Type of HQP Training and Status	Years Supervised or Co-supervised	Title of Project or Thesis	Present Position
Consent Received from Marie Roy				
Roy, Marie	Undergraduate (Completed)	Supervised 1994 - 1997	Isotope geochemistry in petroleum engineering	V-P (Research), Earth Analytics Inc., Calgary, Alberta
Consent Not Obtained from Marie Roy				
(name withheld)	Undergraduate (Completed)	Supervised 1994 - 1997	Isotope geochemistry	research executive in petroleum industry - western Canada

Consent Form

Name of Trainee	
Applicant Information	
Name	
Department	Postsecondary Institution
<p>I hereby allow the above-named applicant to include limited personal data about me in grant applications submitted for consideration to NSERC for the next six years. This limited data will only include my name, type of HQP training and status, years supervised or co-supervised, title of the project or thesis and, to the best of the applicant's knowledge, my position title and company or organization at the time the application is submitted. I understand that NSERC will protect this data in accordance with the <i>Privacy Act</i>, and that it will only be used in processes that assess the applicant's contributions to the training of highly qualified personnel (HQP), including confidential peer review.</p>	
_____ Trainee's signature	_____ Date
Note: This form must be retained by the applicant and made available to NSERC upon request.	

Project #1

Supervisor: J. DONALDSON

Co-supervisor (if any):

Office: SW 632A

Sub-discipline: Phys / Environ Chem

Laboratory: TRACES

Course code: CHM D90/91

e-mail: jdonalds@utsc.utoronto.ca

of students: 1

Web:

CAN WE MEASURE HYDROGEN BONDING TO SOLVENT USING RAMAN SPECTROSCOPY?

Abstract

Dissolved halide anions are known to perturb the intensities and shapes of the bands in the Raman spectra of water (both the OH stretching and the HOH bending modes) and some alcohols. As well, there have been some studies that have measured new, low-energy vibrations in the spectra of aqueous halide solutions; these have been assigned to hydrogen bonding between the anion and the solvating water molecules. This project will investigate the influence of a suite of dissolved anions on the Raman spectra of small alcohols, acetone, DMSO and mixtures of these with water, to look for trends in hydrogen bonding as a function of anion and cation identity. The experimental results will be analysed using simple models for vibrational spectra, and perhaps using quantum chemical methods.

- Learning outcomes. Students will gain experience in a (directed) independent research project whose outcome is not known beforehand. Specific experience will be gained in using modern Raman spectrometers and the analysis of spectroscopic data and the accurate and careful preparation of solutions.
- Required training certificates. Students will need to be trained in the use of the instrument and have access to TRACES.
- Our expectations from student. The student will meet weekly with the supervisor, discuss results and devise an updated plan for work. Student will prepare the appropriate solutions, measure their Raman spectra, save the results and create appropriate plots and analyses. The student will prepare (with some editorial guidance from the supervisor) a final report.

References for further reading

Hidaka et al., *J. Solution Chem.* **2003**, 32, 239-251.

Rull, *Pure Appl. Chem.*, **2002**, 74, 1859–1870.

Heisler et al., *J. Phys. Chem. B* **2011**, 115, 1863–1873

Project #2

Supervisor: J. DONALDSON

Co-supervisor (if any):

Office: SW 632A

Sub-discipline: Phys / Environ Chem

Laboratory: TRACES

Course code: CHM D90/91

e-mail: jdonalds@utsc.utoronto.ca

of students: 1

CAN WE TRACK OXIDATION OF DOM SPECTROSCOPICALLY?

Abstract

Dissolved organic matter (DOM), generally formed from biogenic material, is pretty ubiquitous in natural fresh and salt water systems. Such compounds, when they absorb solar radiation, can produce oxidizing species, such as OH and singlet oxygen, in solution. Although there are many different compounds involved, and thus spectral characteristics, there is often a distinctive region in the excitation – emission spectral maps that is assigned to common DOM chromophores. A recent report has shown that the spectral map of DOM exposed to photogenerated OH oxidant shows differences from the parent map. The purpose of this study is to explore and try to quantify this effect, to determine whether there is a way to infer oxidative lifetime (that is, how long the DOM has been exposed to oxidants) through excitation – emission maps.

- Learning outcomes. Students will gain experience in a (directed) independent research project whose outcome is not known beforehand. Specific experience will be gained in using modern Raman spectrometers and the analysis of spectroscopic data and the accurate and careful preparation of solutions.
- Required training certificates. Students will need to be trained in the use of the instrument and have access to TRACES.
- Our expectations from student. The student will meet weekly with the supervisor, discuss results and devise an updated plan for work. Student will prepare the appropriate solutions, measure their excitation and emission spectra, save the results and create appropriate plots (the excitation – emission maps) and analyses. The student will prepare (with some editorial guidance from the supervisor) a final report.

References for further reading

Jee et al., *Water Sci. Technol.* **2010**, 65, 340 – 346.

Project #7

Supervisor: **Artur Izmaylov**

Office: **SW638**

Laboratory: **SW638**

e-mail: artur.izmaylov@utoronto.ca

Web: <http://www.uts.utoronto.ca/~aizmaylov/>

Co-supervisor: **N/A**

Sub-discipline: **Theoretical/Computational**

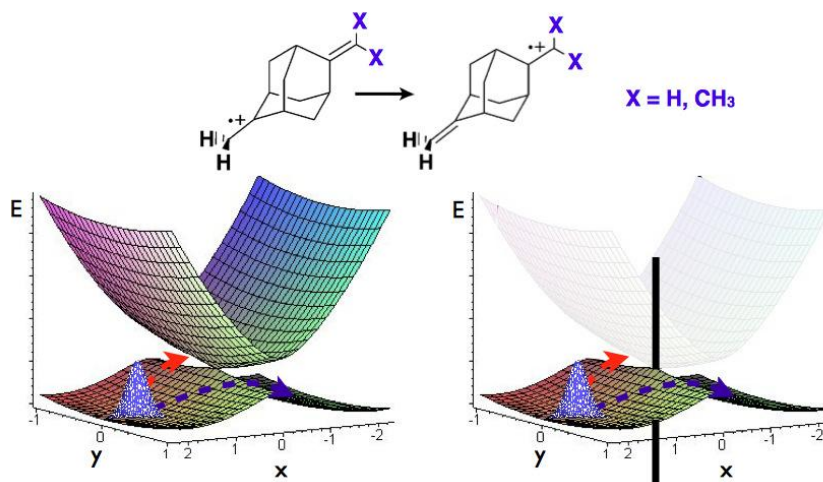
Course code: **CHMD90/91**

of students: **1**

GEOMETRICAL PHASE EFFECTS IN MOLECULAR CHARGE TRANSPORT

Usual physical properties of molecules (e.g., electronic spectra, vibrational frequencies, NMR shifts) are defined by details of potential energy surfaces (PESs). Surprisingly, there also exist measurable properties that appearing because of global geometry of PES rather than its details. The difference between global geometry and local details can be illustrated considering simple geometric objects like torus and sphere: they are very similar if we focus on their small parts but have very different overall shape. In this project we will investigate geometrical phase effects originating in some charge transfer reactions because of nontrivial intersection geometry of donor / acceptor PESs.

- A student working on this project will gain experience in modeling quantum chemistry.
- This project requires basic knowledge of physical chemistry and calculus. Programming experience is preferable but not crucial.
- Student is expected to present the research results in weekly group meetings



References:

- [1] C. A. Mead and D. G. Truhlar, **J. Chem. Phys.** **70**, 2284 (1979)
- [2] A. Shapere and F. Wilczek, **Geometric Phases in Physics** (1989)

Project #8

Supervisor: **Artur Izmaylov**

Co-supervisor: **N/A**

Office: **SW638**

Sub-discipline: **Theoretical/Computational**

Laboratory: **SW638**

Course code: **CHMD90/91**

e-mail: artur.izmaylov@utoronto.ca

of students: **1**

Web: <http://www.uts.utoronto.ca/~aizmaylov/>

FIRST STEP IN VISION: QUANTUM DYNAMICS STUDY

The first step in vision process regulated by the rhodopsin protein involves photo-induced dynamics that starts with the retinal chromophore isomerization from the 11-cis to the all-trans form. Two electronic states are involved in this photochemical process, and therefore, it is necessary to go beyond the Born-Oppenheimer approximation to build an adequate model of this process. Recently, more accurate potential electronic surfaces (PESs) have become available, and in this project we will build correlations between topography of PESs and the photochemical yield: the ratio between the 11-cis and all-trans forms. To build such correlation we will simulate quantum dynamics starting with a minimal but adequate model of two electronic surfaces and two nuclear coordinates. Future extensions of this work will investigate adding more nuclear degrees of freedom, and differences in dynamics stimulated by coherent (laser) and incoherent (sun) light sources.

- A student working on this project will gain experience in quantum mechanical modeling of biological processes using methods of quantum dynamics.
- This project requires basic knowledge of physical chemistry and calculus. Programming experience is preferable but not crucial.
- Student is expected to present the research results in weekly group meetings

References:

[1] I. Schapiro et al., **J. Am. Chem. Soc.** **133**, 3354 (2011)

Project #9

Supervisor: **Artur Izmaylov**

Office: **SW638**

Laboratory: **SW638**

e-mail: artur.izmaylov@utoronto.ca

Web: <http://www.uts.utoronto.ca/~aizmaylov>

Co-supervisor: **N/A**

Sub-discipline: **Theoretical/Computational**

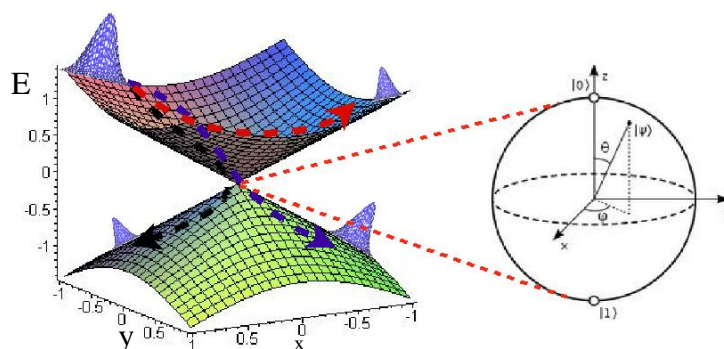
Course code: **CHMD90/91**

of students: **1**

CLASSICAL SPIN FOR PHOTOCHEMICAL REACTIONS

Molecules are very small objects and their behavior is naturally described by quantum mechanics. Quantum mechanics is a more general and more complex theory than the normal, so-called classical mechanics that describes behavior of large objects (e.g., cars and baseballs). Thus, classical mechanics should follow from quantum mechanics when we consider bigger objects. In many chemical reactions involving rearrangement of nuclear fragments that are heavier than hydrogen atom, simple classical description is satisfactory and complex quantum mechanics can be avoided. However, there are many cases, especially in photochemistry, when nuclear motion is not confined to only one potential electronic surface, in other words, the Born-Oppenheimer approximation breaks down, and classical description stops working. Is there a way to avoid complexity of quantum mechanics for such situations? In this project we will employ physical construction of classical spin to represent classically reaction dynamics beyond the Born-Oppenheimer approximation.

- A student working on this project will gain better understanding of quantum-classical correspondence and experience in modeling techniques.
- This project requires basic knowledge of physical chemistry and calculus. Programming experience is preferable but not crucial.
- Student is expected to present the research results in weekly group meetings



References:

- [1] A. Atland and B. Simons, **Condensed Matter Field Theory** (2010)
- [2] V. Krishna, **J. Chem. Phys.** **126**, 134107 (2007)

Project #11

Supervisor: **Kagan Kerman**

Co-supervisor (if any): **M. Simpson**

Office: **SW533**

Sub-discipline: **Bioanalytical Chemistry**

Laboratory: **SW221**

Course code: **CHMD90/91**

e-mail: kagan.kerman@utoronto.ca

of students: **1**

Web: <http://www.utoronto.ca/~kkerman/>

ELECTROCHEMICAL OXIDATION OF DISSOLVED ORGANIC MATTER

Dissolved organic matter (DOM) functions as an intermediate in microbial metabolic processes and facilitate the cycling of multi-oxidation state metals in biogeochemical redox reactions [1]. Quinone functional groups associated with DOM are frequently cited as important organic moieties responsible for the redox activity of inorganic contaminants [2]. Electrochemical study of DOM would lead to a better understanding of the structural components responsible for redox behavior, such as quinones and nitrogen and sulfur (N/S) functional groups [3-5]. This project will utilize voltammetric techniques (differential-pulse, square-wave and stripping) coupled with NMR spectroscopy. DOM isolates from diverse sources will be tested using platinum as well as nanoparticle-modified carbon working electrodes. The electrochemical profiles of DOM will be correlated with the NMR data to understand their structural details and redox-active moieties.

- This project requires a team effort with graduate students, and is co-supervised with Professor Myrna Simpson (DPES, UTSC).
- A student working on this project will gain experience in electroanalytical techniques and NMR spectroscopy.
- Student is expected to present the research results in weekly group meetings (tentatively Friday afternoons).

References:

- [1] Lovley D. R., Coates J. D., Blunt-Harris E. L., Phillips E. J. P., and Woodward J. C. (1996) Humic substances as electron acceptors for microbial respiration. *Nature* 382, 445–448.
- [2] Struyk Z., and Sposito G. (2001) Redox properties of standard humic acids. *Geoderma* 102, 329–346.
- [3] Nurmi J. T., and Tratnyek P. G. (2002) Electrochemical properties of natural organic matter (NOM), fractions of NOM, and model biogeochemical electron shuttles. *Environ. Sci. Technol.* 36, 617–624.
- [4] Fimmen, R. L., Cory, R. M., Chin, Y.-P., Trouts, T. D., McKnight, D. M. (2007) Probing the oxidation-reduction properties of terrestrially and microbially derived dissolved organic matter. *Geochim. Cosmochim. Acta* 71, 3003-3015.
- [5] Tian, M., Wen, J., MacDonald, D., Asmussen, R. M., Chen, A. (2010) A novel approach for lignin modification and degradation. *Electrochem. Commun.* 12, 527-530.

Project #12

Supervisor: **Kagan Kerman**

Co-supervisor (if any):

Office: **SW533**

Sub-discipline: **Bioanalytical Chemistry**

Laboratory: **SW221**

Course code: **CHMD90/91**

e-mail: kagan.kerman@utoronto.ca

of students: **1**

Web: <http://www.utoronto.ca/~kkerman/>

IMMUNOCHIPS FOR AMYLOID-BETA USING ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

Alzheimer's disease (AD) is a progressive and irreversible neurodegenerative dementia marked by substantial impairments to episodic memory and cognitive functions. Approximately 60% of all late-onset cases of dementia are attributed to AD, which is estimated to afflict more than 500,000 Canadians [1][2]. The amyloid cascade hypothesis attributes AD pathogenesis to an imbalance in amyloid-beta (Abeta), a small 4 kDa peptide capable of undergoing spontaneous self-association to form neurotoxic supramolecular assemblies. Notably, soluble oligomers have been identified as the more relevant toxic species of Abeta relative to later stage fibrillar aggregates and has since become a critical target for future drug therapy development.

We will be developing a rapid, disposable electrochemical immunosensor for determination fibril and oligomer distribution over the course of Abeta aggregation. To this effect, conformation-specific antibodies will be immobilized onto the surface of a gold CD electrode to monitor the inhibition of distinct aggregate states. Surface binding events will be determined by impedance spectroscopy, in which antigen-antibody interactions are quantified as a function of charge transfer resistance across the electrode interface. The efficacy of a small library of novel sym-triazine-derived aggregation modulators to reduce toxic oligomer formation will be evaluated. The results are expected to demonstrate the utility of impedimetric immunosensing for comprehensive identification of effective Abeta aggregation modulators.

- This project requires a team effort with graduate students, and is co-supervised with Professor Ian Brown (Biological Sciences, UTSC). Biosafety certificate is required.
- A student working on this project will gain experience in biosensor development using electroanalytical and biological techniques.
- Student is expected to present the research results in weekly group meetings (Friday afternoons).

References: [1] Blennow, K., et al. (2006) Lancet 368, 387-403.[2] Rising Tide: The impact of dementia on Canadian society <www.alzheimer.ca/>

Project #13

Supervisor: Bernie Kraatz

Co-supervisors:

Office: ESCB 5th floor

Sub-discipline: Inorganic/ Biological

Laboratory: ESCB 5th floor

Course code: CHMD90

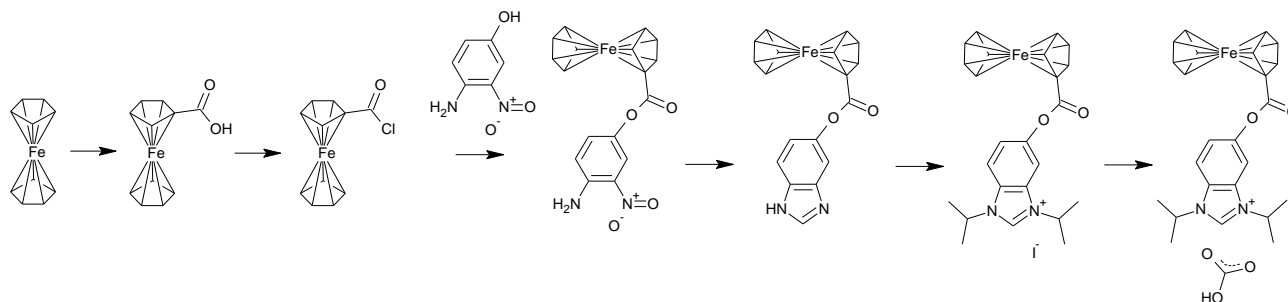
e-mail: bernie.kraatz@utoronto.ca # of students: 1

Web: <http://www.utoronto.ca/~bkraatz/>

Ferrocene-terminated benzimidazole and its derivatives

Carbenes, a class of compounds that have one of the carbon atoms in an oxidation state of two, are known to react with variety of metals forming stable self-assembled monolayers (SAMs) on surfaces. In situ carbene formation from air-stable precursors followed by a reaction with a metal surface may lead to an analogous coat formation. This organic layer covalently bound to a metal may be potentially used as a corrosion protection coat.

The ferrocene is a redox active moiety; as a result, ferrocene based building blocks have already been used successfully in fabrication of various SAMs. Analysis of cyclic voltammograms of ferrocene-terminated SAMs allows determination of the charge involved in the redox process, and thus to calculate actual surface coverage of the ferrocene units.



Ø Learning outcomes: In this project, the student will be involved in the synthesis of various ferrocene-terminated benzimidazole derivatives by solution phase methods, their isolation and characterization by spectroscopic methods (NMR, IR, MS) thus gaining invaluable experience in advanced synthetic and analytical techniques.

Ø Required training certificates WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Project #14

Supervisor: Bernie Kraatz

Co-supervisors:

Office: ESCB 5th floor

Sub-discipline: Inorganic/ Biological

Laboratory: ESCB 5th floor

Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca # of students: 1 -2

Web: <http://www.uts.utoronto.ca/~bkraatz/>

Development of Peptide Co-Gels

Peptide molecules can interact via hydrogen bonding and π -stacking interactions to generate materials that allow the inclusion of large quantities of solvent molecules. In these gels, peptides engage in interactions that exhibit some level of order but lack crystallinity. Our group has studied a series of stimuli-responsive gels in which the gel can react to external stimuli (see references).

This project focuses on co-gels, in which two peptide gelators can interact with each other and generate a wide range of gel properties. This project will explore issues related to co-assembly and to self-sorting. We have reported before the self-sorting behavior of a series of gels that carry a fluorescent label (see references). Here, the gel forming properties of the ferrocene-peptide conjugate Fc-CO-FFL-OMe will be probed. The investigation will involve various diastereomers of this peptide and the gel and co-gelation will be studied using a range of experimental techniques, including circular dichroism, ¹H-NMR, and IR spectroscopies. In addition, variable temperature NMR spectroscopy is ideal for the study of intermolecular H-bonding interactions. Morphologies of the gels will be studied by electron microscopy.

R. Afrasiabi, H.B. Kraatz, *Chem. Eur. J.* **2015**, *21*, 7695-7700; B. Adhikari, H.-B. Kraatz, *Chem. Commun.* **2014**, *50*, 5551-5553 and references therein.

Ø Learning outcomes: In this project, the student will be involved in the synthesis of various ferrocene-peptide derivatives by solution peptide coupling methods, their isolation by column chromatography and characterization by spectroscopic methods (CD, NMR, IR, MS) thus gaining invaluable experience in advanced synthetic and analytical techniques.

Ø Required training certificates WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Project #15

Supervisor: Bernie Kraatz

Co-supervisors:

Office: ESCB 5th floor

Sub-discipline: Inorganic/ Biological

Laboratory: ECSB 5th floor

Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca

of students: 1

The influence of benzimidazolium hydrogen carbonates on formation of nanostructured silver surfaces

Carbenes, molecules containing a neutral carbon atom with a valence of two and two unshared valence electrons, are known to react with variety of metal ions and metals forming stable metal complexes or self-assembled monolayers (SAMs) on metal surfaces. However anhydrous conditions and inert atmosphere are required for carbenes in their so called “free carbene” form. Alternatively air-stable carbene precursors could be utilized for the same purposes. We plan to elaborate and optimize a method for the formation of stable carbene based SAMs at ambient conditions.

This project will start with synthesis of several benzimidazolium based carbene precursors and formation of SAMs on silver surfaces. Electrochemical cycling of these SAM-covered silver surfaces in aqueous solutions will be performed to get an idea of stability of the SAMs. Further electrochemical cycling of SAM- functionalized silver surfaces in solutions of carbene precursors in organic solvents will be performed to track changes in the electrochemical response due to either disruption of the original SAM layer, or due to the formation of silver nanostructures. Since carbene precursors may form either homogeneous silver complexes or react directly with a surface of a metal cluster, electrochemical cycling may result in silver leaching from the surface followed by the formation of silver complexes in solution. Alternatively, it may result in the formation of metal clusters followed by their deposition on the surface. These clusters on silver surfaces may be potentially useful for sensing applications in biomedical sciences or pollution monitoring.

Ø Learning outcomes: Student participating in this project will be involved in the synthesis of various benzimidazole derivatives by solution phase methods, their isolation and characterization by spectroscopic methods (NMR, IR, MS) thus gaining invaluable experience in advanced synthetic and analytical techniques. In addition, the student will get valuable experience in the formation of SAMs, their characterization (XPS and e-chem stripping), and surface modification by e-chem cycling.

Ø Required training certificates: WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all

group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Project #16

Supervisor: Bernie Kraatz

Co-supervisors:

Office: ESCB 5th floor

Sub-discipline: Inorganic/ Biological

Laboratory: ECSB 5th floor

Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca

of students: 1

Pathogen detection by electrochemical methods

The objective of this project is to study the electrochemical behaviour of modified surfaces and their interactions with pathogenic agents. My group has studied biosensing surfaces for a wide range of bioanalytes, including DNA. In previous studies, electrochemical studies of DNA-modified gold micro-electrodes allowed us to distinguish mismatched positions and mismatch pairs of DNA, as well as being able to distinguish between mitochondrial DNA fragments in the cytochrome C1 oxidase gene (see references).

In this study, different bio-recognition elements, such as DNA and antibody proteins, will be investigated towards detection whole bacteria and pathogen-associated molecular patterns, such as for *Escherichia coli* and *Salmonella*, which are commonly found in our lake water and in contaminated meats.

The approach will be carried out in this project is to combine surface chemistry with electrochemistry. Bio-recognition elements will be immobilized onto gold surfaces and their bindings to the targets will be monitored using Cyclic Voltammetry, Square Wave Voltammetry and Electrochemical Impedance Spectroscopy. The aim is to develop biosensors that are able to convert biological responses into sensitive quantifiable electric signals and construct calibration curves for the biological targets

Diakowski, P. M.; Kraatz, H.-B. *Chem. Commun.* **2009**, 1189; Shamsi, M. H.; Kraatz, H.-B. *Analyst* **2010**, *135*, 2280; Shamsi, M. H.; Kraatz, H. B. *Analyst* **2011**, *136*, 4724; 3107; Diakowski, P. M.; Kraatz, H. B. *Chem. Commun.* **2011**, *47*, 1431.

Ø Learning outcomes: Student will be involved in the modification of surfaces, their characterization by spectroscopic and electrochemical methods and their interactions with bioanalytes and the construction of response curves.

Ø Required training certificates: WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Drs. Iralkii Ebralidze and Zhe She and graduate students.

Project #17

Supervisor: Bernie Kraatz

Co-supervisors:

Office: ESCB 5th floor

Sub-discipline: Inorganic/ Biological

Laboratory: ECSB 5th floor

Course code: CHMD90

e-mail: bernie.kraatz@utoronto.ca # of students: 1

Study of metal ion interactions with peptides.

The protein Tau is responsible for microtubule stabilization in neuronal cells and their activity is regulated by kinase-catalyzed phosphorylations. Hyperphosphorylation of Tau causes catastrophic destabilization of the microtubules, followed by assembly of phosphorylated Tau into neurofibrillar tangles on the interior of the neuronal cells causing cell death. Metal ions are found to be associated with these neurofibrillary protein tangles.

This project focuses on the study of a range of metal ions (Fe^{3+} , Cu^{2+} etc) with peptide fragments of Tau. We have evaluated phosphorylations and Cu^{2+} binding to full length Tau before and studied its behavior by electrochemical and spectroscopic means (see references). This project will focus on solution studies involving Tau peptides and metal ions. The interactions will be monitored by calorimetry, which will allow the evaluation of the thermodynamics of the interaction, and by circular dichroism spectroscopy, which will allow probing structural changes as a result of the interaction.

S. Martić, M.K. Rains, H.-B. Kraatz, *Anal. Biochem.* **2013**, 442, 130-137; S. Martić, S. Beheshti, M. K. Rains, H.-B. Kraatz, *Analyst* **2012** 137, 2042-2046.

Ø Learning outcomes: Student will be involved in the calorimetric and CD spectroscopic studies and their evaluation and learn basic bioinorganic techniques.

Ø Required training certificates: WHMIS

Ø Our expectations from students: I expect students to work effectively and collaboratively with graduate students and postdoctoral fellows and fully participate in all group activities and meetings. I expect monthly written updates on progress. Weekly meetings with the supervisor will be arranged. Day-to-day interactions with Soha Ahmadi.

Project #18

Joint Supervisor: **Andre Simpson** Joint Supervisor: **Xiao-an Zhang**

Office: **SY324** Sub-discipline: **Organic/Analytical/Environmental**

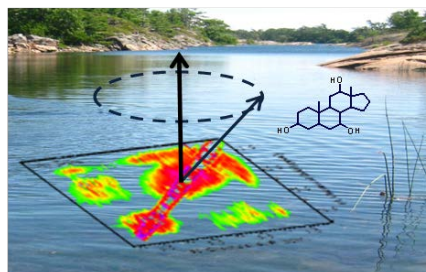
Laboratory: **SY050** Email: andre.simpson@utoronto.ca and xazhang@utsc.utoronto.ca

NMR Anion Sensors, Functional Group Capping and Mass Spectrometry: A multidisciplinary approach to address the world's most complex mixture.

Dissolved Organic Matter (DOM) is ubiquitous in all natural waters and known to play important roles in the global carbon and nitrogen cycles, the fate, transport and transformation of contaminants and nutrients and the health and biodiversity of aquatic species. DOM, however, is not just important due to its key role in environmental processes but its structural signatures themselves of immense interest. This is probably best summarized by John Hedges, arguably one of the greatest oceanographers of the modern era, he stated, "*The 10^{12} diverse organic molecules dissolved in every milliliter of seawater are the only constituents whose stored information approaches the richness needed to understand where the water has been and what has happened within it over time. The future of oceanographic research belongs in part to those who can learn to read these molecular messages.*"

Recently the A. Simpson group through hyphenation of 2D HPLC and 3D NMR has discovered the main constituents of DOM are highly oxygenation terpenoids. However, the analysis took 2 years making it impractical for routine applications. Theoretically if the material could be derivatized such that it can be dissolved in non-polar solvents, high resolution GC-MS methods should be ideal for rapid routine screening of the material. Simple derivatization is not easy as there are many acid and alcohol groups per terpenoids structure and steric hindrance may be problematic when trying to cap all of them. The Zhang group have developed a unique NMR based anion sensor. The sensor works in organic solvents and provides a simple and rapid indicator as to how many unexposed polar groups remain after derivatization.

The project will be a 50:50 collaboration between the A. Simpson and Zhang research groups. The student will attempt various derivatizations (mainly methylations) in the Zhang group and then compare the effectiveness of each approach using the NMR sensor with the A. Simpson group. Finally GC-MS analysis will be performed to assess the additional information provided by more complete derivatization of the materials.



Learning outcomes

- (1) Various organic reactions and derivatization.
- (2) Advanced NMR and NMR sensors.

(3) Gas Chromatography – Mass Spectrometry Analysis.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a scientific publication, we expect the student to be highly involved and lead this process.

Project #21

Supervisor:	Xiao-an Zhang	Co-supervisor (if any):	N/A
Office:	SW511	Sub-discipline:	Organic & Biological Chemistry
Lab:	SW332	Course code:	CHMD90
e-mail:	xazhang@utsc.utoronto.ca	# of students:	1~2
Web:	http://www.utsc.utoronto.ca/~xazhang/		

DEVELOPMENT OF Gd-FREE HIGH RELAXIVITY MRI CONTRAST AGENT

Magnetic resonance imaging (MRI) is a powerful and versatile biomedical imaging modality that is increasingly applied for clinical diagnosis, owing to its noninvasiveness, high resolution, deep penetration and capability of 3-dimensional real-time scans. Conventional MRI relies on the ^1H -NMR signal of water, the most abundant molecule *in vivo*. MRI contrast agent (CA) is a new class of pharmaceuticals that can improve contrast and sensitivity of MRI. Current FDA-approved clinical MRI CAs are predominantly based on low-molecular-weight Gd(III)-complexes, which can enhance the MRI contrast via shortening the longitudinal relaxation time (T_1) of water proton. These Gd T_1 agents, however, typically exhibit relatively low relaxivity (the efficiency of relaxation enhancement), in particular at high magnetic field. Grams-quantities of Gd-agents are required *in vivo* in order to obtain satisfactory imaging effect. Higher dose is unavoidably associated with higher risk of side effects. Recently, several Gd CAs have been implicated in nephrogenic systemic fibrosis (NSF), a severe side effect related to Gd toxicity in patients with renal dysfunction. Therefore, safer and more efficient MRI CAs are highly desirable. This D90 project will be part of our research program in developing next generation MRI T_1 CAs with high relaxivity and low toxicity. The primary goal is to design, synthesize and characterize novel Gd-free agents.

Learning outcomes

- Students will receive hands-on trainings on advanced organic and inorganic synthesis, and are expected to do chemical synthesis independently after training;
- Students will receive trainings on how to use modern spectroscopy techniques, including NMR, ESI-MS, UV-vis, etc to characterize the synthetic intermediates and final product;
- Students will learn background knowledge on MRI contrast agents and explore theory about relaxivity.
- Students are expected to present their research results in group meetings.

Required training certificates

(1) WHMIS training; (2) Chemical Safety Training; Our expectations from students...

- (1) Successfully completed CHMC41 or 42; (2) Previous experience in organic synthesis is preferred.

References: [1] Merbach, A. E.; Tóth, É., *The chemistry of contrast agents in medical magnetic resonance imaging*. Wiley: Chichester ; New York, 2001 [2] Zhang, X.-a.; Lovejoy, K. S.; Jasanoff, A.; Lippard, S. J, *Proc. Natl. Acad. Sci. USA* 2007, 104 (26), 10780.

Project #22

Supervisor:	Xiao-an Zhang	Co-supervisor (if any):	N/A
Office:	SW511	Sub-discipline:	Organic & Biological Chemistry
Lab:	SW332	Course code:	CHMD90
e-mail:	xazhang@utsc.utoronto.ca	# of students:	1~2
Web:	http://www.utsc.utoronto.ca/~xazhang/		

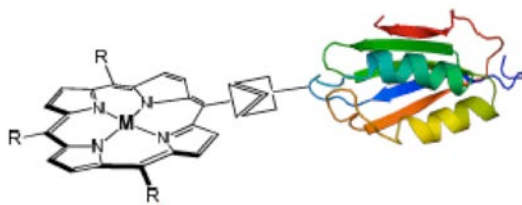
DESIGN AND SYNTHESIS OF MRI CONTRAST AGENT FOR COVALENT PROTEIN LABELING

Molecular imaging probes, including fluorophores, radioactive tracers, or magnetic resonance imaging (MRI) contrast agents (CAs) that can be selectively attached to specific bio-macromolecules, such as proteins, are powerful and versatile research tools for molecular biology as well as for medical diagnosis. These biomedical imaging probes can be used to label and track the selected protein targets inside the biological system to provide their distribution kinetics and functional information. On the other hand, certain proteins, such as antibody, can be used as a cargo to deliver imaging probes to specific sites, such as surface of tumor cells.

This project aims to develop novel MRI contrast agents based on water-soluble porphyrins for protein labeling. MRI is one of the major medical imaging modalities that is increasingly used for clinical diagnosis. The immediate goal of current project is to establish a synthetic strategy with reasonable yield and to structurally characterize the final product.

Learning outcomes

- Students will be systematically trained on organic and inorganic synthesis, in particular on porphyrin synthesis;
- Students will receive hands-on trainings on how to use modern spectroscopy techniques, including NMR, ESI-MS, UV-vis, etc to characterize the synthetic intermediates and final product;
- Students will learn background knowledge on MRI contrast agents, molecular imaging and molecular design.
- Student is expected to present the research results in group meetings.
- Required training certificates: (1) WHMIS training; (2) Chemical Safety Training; Our expectations from students...
- Successfully completed CHMC41 or 42; (2) Previous experience in organic synthesis is preferred.



References: [1] Merbach, A. E.; Tóth, É., *The chemistry of contrast agents in medical magnetic resonance imaging*. Wiley: Chichester ; New York, 2001 [2] Zhang, X.-a.; Lovejoy, K. S.; Jasanoff, A.; Lippard, S. J, *Proc. Natl. Acad. Sci. USA* 2007, 104 (26), 10780.

Project #23

Supervisor: Ronald Soong

Co-supervisor (if any): Andre Simpson

Office: SY324 Sub-discipline: Analytical/Biological

Laboratory: SY050

Course code: CHMD90

e-mail: ronald.soong@utoronto.ca

of students: 1

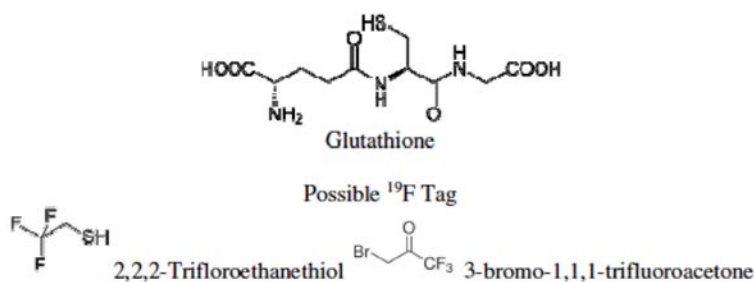
Web: <http://www.utoronto.ca/~asimpson/>

¹⁹F TAGGING OF THIOLS AS AN APPROACH FOR THE NMR DETECTION AND QUANTIFICATION OF GLUTATHIONE AND ITS DERIVATIVES IN BIOFLUIDS

Glutathione and its derivatives are important biomarkers in the measurement of oxidative stress in an organism. Therefore, significant amount of work has been done for the detection and qualification of glutathiones in various biofluids, such as blood, urine and tissue extracts. Nuclear Magnetic Resonance (NMR) NMR spectroscopy is one of the most powerful tools for studying metabolite fluxes in intact biofluids. However, for most complex biological fluids the ¹H NMR resonances of glutathiones are often indistinguishable from other metabolites due to severe spectral overlap. However, the thiol (SH) group can be activated to form disulfide bonds, allowing us to add NMR observable ¹⁹F tag for detection. ¹⁹F tag offers several advantages, including 100% natural abundance and highly sensitive to its chemical environment. The goal of this D90 project is to investigate various strategies in incorporating different ¹⁹F tag through disulfide bond linkage in standard Glutathiones and in biological tissue extracts.

Learning outcomes :

- Hands-on-experience and training with state-of-art NMR spectroscopy. Experience with the derivatization of biological molecules. Experience in metabolomics (one of the most powerful approaches to understand biological response).
- Required training certificates : WHMIS
- Our expectations from students. Hard working, open minded student, with interests in more than one area of chemistry. Ambition to publish results in a top international journal.



References

- Potapenko, D.I. et al. *Magn. Reson. Chem.*, **43** (2005) 902–909
Loewen. M.C. et. al. *Proc. Natl. Acad. Sci. USA*, **98** (2001) 4888–4892.

Project #24

Supervisor: F. WANIA

Co-supervisor (if any):

Office: SY 364

Sub-discipline: Environ Chem

Laboratory: SY370

Course code: CHM D90/91

e-mail: frank.wania@utoronto.ca

of students: 1

Predicting Phase Partitioning Equilibria of the Oxidation Products of Volatile Organic Compounds Involved in Secondary Organic Aerosol Formation

In order to understand the growth of organic particles in the atmosphere and the yield of secondary organic aerosol (SOA) formation, it is necessary to know the equilibrium partition coefficients between aerosol and gas phase at different temperatures for a large number of atmospheric oxidation products. Experimental values for these partition coefficients are missing for most of the chemicals involved in SOA formation, because many of them have not even been synthesized. In fact, many of their physico-chemical properties are missing and need to be predicted with methods of variable complexity and sophistication. Examples are the poly-parameter linear free energy relationship (ppLFER) approach, the SPARC (SPARC Performs Automated Reasoning in Chemistry) software, and the CONductor like Screening MOdel for Realistic Solvents (COSMO-RS). The project involves the identification of the relevant oxidation products, the conversion of their molecular structure into a format that can be read by computer programs, the prediction of partitioning properties and their illustration and interpretation.

- Learning outcomes. Students will gain experience in a (directed) independent research project whose outcome is not known beforehand. Specific experience will be gained in using chemical property prediction software.
- This project requires basic knowledge of physical chemistry.
- Our expectations from student. The student will meet weekly with the supervisor, discuss results and devise an updated plan for work. The student will prepare (with some editorial guidance from the supervisor) a final report.

References:

Hallquist, M., et al.: The formation, properties and impact of secondary organic aerosol: current and emerging issues, *Atmos. Chem. Phys.*, 9, 5155–5236, doi:10.5194/acp-9-5155-2009, 2009

Supervisor: **Ronald Soong**

Co-advisor: **Artur Izmaylov**

Office: **SW155B**

Sub-discipline: **Instruments**

Laboratory:

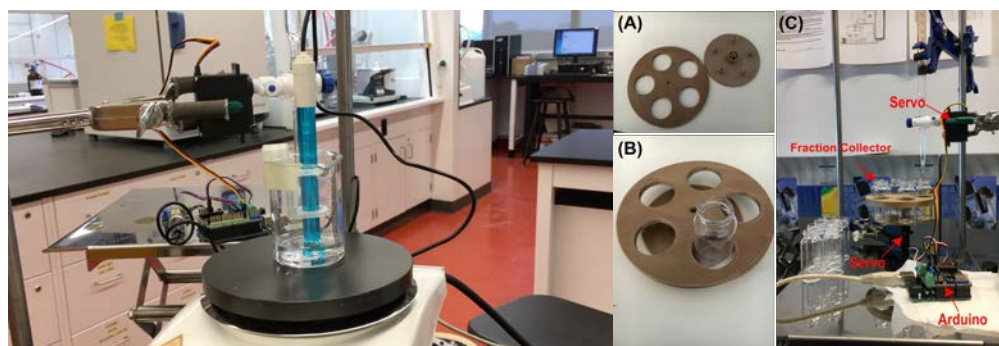
Course code: **CHMD90/91**

e-mail: ronald.soong@utoronto.ca

of students: **1**

Construction and Evaluation of Portable Analytical Instruments Based on the Arduino Microcontroller

A microcontroller is a micro-computer that is small and generally inexpensive. They are low-powered and can be powered through a variety of ways, including a USB connection, a wall socket, and a 9V battery¹. Several types of microcontrollers are commercially available; the specific microcontroller studied here is called the Arduino. In this project, the student will be tasked with designing and making analytical instruments for undergraduate experiments. The goal is to create these low cost instruments such that they are affordable. The student is encourage to be creative while applying their knowledge in chemistry. The instruments that the student will be building will be 1) An auto-titrator 2) A cellphone spectrophotometer 3) auto-pipeter. Through designing and making these instruments, the student will gain hand-on experience with microelectronics and engineering in addition to basic analytical chemistry.



co-supervisor: **Ronald Soong**

Sub-discipline: Analytical/Biological

Course code: **CHMD90**

Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

Investigating ^{15}N as an important nucleus to better understand biochemical processes through *in-vivo* NMR

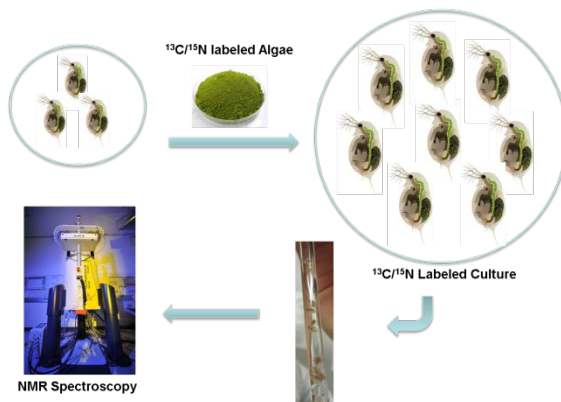
D. magna are the standard organism used globally for aquatic toxicity testing. The present method used by regulatory bodies to assess aquatic toxicity of a compound is the “21 day reproducibility test”. If no perturbations are noted in reproducibility then the chemical is deemed to be safe at that concentration. However, the literature has repeatedly reported more subtle effects such as DNA damage, changes to metabolic pathways, bioaccumulation, permanent binding can be missed using this standard approach as such there is great need to develop more informative, sensitive and rapid methods to truly evaluate aquatic toxicity.

In-vivo NMR, has the potential to monitor not only the entire molecular fingerprint of an organism in real time but also relates changes in the molecular profile to uptake, transformation, binding, bio-concentration and secretion of a contaminant species. As such *in-vivo* NMR provides the technical framework required to understand “how” and “why” certainly chemicals are toxic, information desperately needed by regulators to set more meaningful standards. Despite its considerable potential *in-vivo* NMR has not yet been applied to evaluate toxicity in an environmental context.

Optimizing the depth and variety of information that can be obtained via *in-vivo* NMR will be critical to comprehensively evaluate toxic pathways. With this in mind ^{15}N NMR (1D and multidimensional) will be explored as a potentially powerful tool to study metabolites, proteins and other biomolecules *in-vivo*. Organisms will be fed a diet of ^{15}N labelled algae and various NMR schemes will be developed to observe and differentiate metabolites and macromolecules *in-vivo*. It is anticipated ^{15}N labelling will provide a wealth of novel information complimentary to common NMR studies focusing on ^1H and ^{13}C .

Learning outcome

- (1) The student will receive hands-on training on culturing and isotopic labelling *D. Magna*
- (2) The student will receive training on using advanced NMR spectroscopy required for *in-vivo* studies.
- (3) The student will learn about different statistical methods for data analysis and interpretation.



Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a co-authored scientific publication, we expect the student to be involved in this process as required.

Supervisor: **Andre Simpson**

co-supervisor: **Ronald Soong**

Office: **SY324**

Sub-discipline: **Analytical/Biological**

Laboratory: **SY050**

Course code: **CHMD90**

Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

Investigating ^{31}P as an important nucleus to better understand energetic processes through *in-vivo* NMR

D. magna are the standard organism used globally for aquatic toxicity testing. The present method used by regulatory bodies to assess aquatic toxicity of a compound is the “21 day reproducibility test”. If no perturbations are noted in reproducibility then the chemical is deemed to be safe at that concentration. However, the literature has repeatedly reported more subtle effects such as DNA damage, changes to metabolic pathways, bioaccumulation, permanent binding can be missed using this standard approach as such there is great need to develop more informative, sensitive and rapid methods to truly evaluate aquatic toxicity.

In-vivo NMR, has the potential to monitor not only the entire molecular fingerprint of an organism in real time but also relates changes in the molecular profile to uptake, transformation, binding, bio-concentration and secretion of a contaminant species. As such *in-vivo* NMR provides the technical framework required to understand “how” and “why” certainly chemicals are toxic, information desperately needed by regulators to set more meaningful standards. Despite its considerable potential *in-vivo* NMR has not yet been applied to evaluate toxicity in an environmental context.

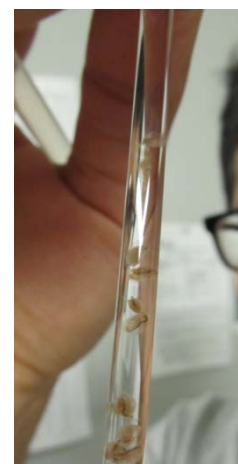
Optimizing the depth and variety of information that can be obtained via *in-vivo* NMR will be critical to comprehensively evaluate toxic pathways. With this in mind ^{31}P NMR (1D and multidimensional) will be explored as a potentially powerful tool to study metabolites (such as ADP, ATP, phospholipids etc.) and biomolecules RNA/DNA *in-vivo*. Organisms will studies *in-vivo* and *in-vitro* after chemical extraction. High resolution NMR from extracts will be useful for assignments of broader signal in ^{31}P *in-vivo* NMR. It is anticipated ^{31}P NMR provide a wealth of novel information complimentary to common NMR studies focusing on ^1H and ^{13}C .

Learning outcome

- (1) The student will receive hands-on training on culturing *D. Magna*
- (2) The student will learn various extraction approaches.
- (3) The student will receive training on using advanced NMR spectroscopy required for *in-vivo* studies.
- (4) The student will learn about different statistical methods for data analysis and interpretation.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a co-authored scientific publication, we expect the student to be involved in this process as required.



Supervisor: **Andre Simpson**

co-supervisor: **Ronald Soong**

Office: **SY324**

Sub-discipline: **Analytical/Biological**

Laboratory: **SY050**

Course code: **CHMD90**

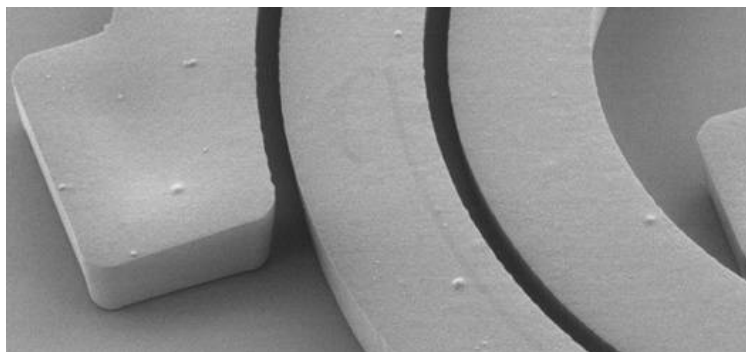
Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

The Application and Development of Micro Surface Coil NMR.

NMR spectroscopy is arguably the most powerful tool in modern research with the ability to provide unprecedented levels of information regarding molecular structure and interactions. However, the relatively low sensitivity of NMR is its main drawback. Recently, new nanolithography techniques allow the “printing” of NMR coils as small as individual cells. Such coils provide theoretical mass sensitivities ~50 times higher or time savings of ~2500 times in comparison to conventional NMR technology.

However, when moving to such small samples questions become: “how do we handle such samples?”, “how do we retain the sample on the coil?”, “how do we prevent evaporation?”, “can organisms be kept alive on these coils?”, “how small can we go?”, and “what are applications of coils of varying diameter?”

The D90 student will work alongside graduate students and PI's to assist in answering these questions. The student will be immersed in all areas of the project and will learn a diverse array of techniques, application and theory. The student will test various applications that include plants, cells, organisms, tissue, small fruits/seeds. In both static and flow orientations.



Learning outcome

- (1) The student will receive hands-on training on handling tiny samples using microscopes.
- (2) The student will receive training on using advanced NMR spectroscopy, including advanced water suppression, advanced acquisition and spectral interpretation approaches.
- (3) The student will learn about theory and application of cutting edge, globally unique, micro-coil NMR technology.
- (4) The student will work with a diverse range of chemical, environmental and biological samples.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry. It is highly likely the work will lead to a co-authored scientific publication, we expect the student to be involved in this process.

Supervisor: **Andre Simpson**

co-supervisor: **Ronald Soong**

Office: **SY324**

Sub-discipline: **Analytical/Biological**

Laboratory: **SY050**

Course code: **CHMD90**

Email: andre.simpson@utoronto.ca and ronald.soong@utoronto.ca

Understanding real-time bioaccumulation and transformation of perfluorinated contaminants in *Daphnia magna* using *in-vivo* NMR

D. magna are the standard organism used globally for aquatic toxicity testing. The present method used by regulatory bodies to assess aquatic toxicity of a compound is the “21 day reproducibility test”. If no perturbations are noted in reproducibility then the chemical is deemed to be safe at that concentration. However, the literature has repeatedly reported more subtle effects such as DNA damage, changes to metabolic pathways, bioaccumulation, permanent binding can be missed using this standard approach as such there is great need to develop more informative, sensitive and rapid methods to truly evaluate aquatic toxicity.

In-vivo NMR, has the potential to monitor not only the entire molecular fingerprint of an organism in real time but also relates changes in the molecular profile to uptake, transformation, binding, bio-concentration and secretion of a contaminant species. As such *in-vivo* NMR provides the technical framework required to understand “how” and “why” certainly chemicals are toxic, information desperately needed by regulators to set more meaningful standards. Despite its considerable potential *in-vivo* NMR has not yet been applied to evaluate toxicity in an environmental context.

In this project *in-vivo* NMR will be used to monitor the real time uptake, biotransformation and binding of perfluorinated contaminants which are now found ubiquitously in our environment. Perfluorinated hydrocarbons are present in human blood in the ppb range (50 ppb average in the public) to ppm range (3M workers). The chemicals exhibit complex toxicity that is not well understood. NMR has a key role to play in understanding the toxicity of PFC's for example our group showed that PFOA and PFOS interact preferentially and irreversibly with Sudlow's site I and II on human serum albumin when introduced to human blood. However, at present there have been no studies of PFC's *in-vivo*. The chemicals themselves will be monitored by a range of NMR approaches to understand and explain their biological uptake, accumulation, transformation and secretion. *In-vivo* NMR holds great potential to understand the impact of chemicals prior to mass release into the environment.

Learning outcome

- (1) The student will receive hands-on training on culturing *D. Magna*
- (2) The student will receive training on using advanced NMR spectroscopy required for in-vivo studies.
- (3) The student will learn about different statistical methods for data analysis and interpretation.

Required Training: WHMIS

Our expectation from students: Hard working, open minded student, with interests in more than one area of chemistry.

Supervisor: Ruby Sullan

Office: EV566

Laboratory: EV 506-523

e-mail: ruby.sullan@utoronto.ca

Web: <http://www.utoronto.ca/physsci/ruby-sullan>

Co-supervisor (if any): NA

Sub-discipline: Biophysical Chemistry

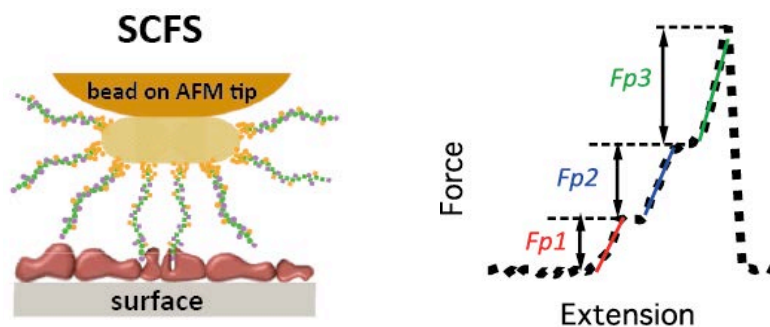
Course code: CHMD90/91

of students: 1

**Interaction forces between *E. coli* and PDMS substrates of varying stiffness:
Single cell force spectroscopy**

Central to the initiation and maturation of biofilms are the bacterial cell surface adhesion molecules (adhesins) that mediate initial attachment between the cell and a wide range of surfaces. The chemical nature of these surfaces as well as the biochemical characteristics of the adhesins has been a focus of numerous studies. An important gap that remains to be filled is how bacterial adhesion depends on the stiffness of the underlying substrate. Nothing is currently known about the underlying molecular mechanisms and mechanical forces that govern this substrate-stiffness dependent bacterial adhesion. The goal of this CHMD90/91 research project is to quantify the interaction forces between *E. coli* (wild-type and knockout mutants) and polydimethylsiloxane (PDMS) substrates of varying stiffness using atomic force microscopy (AFM)-based single cell force spectroscopy (SCFS). This will quantify the degree of contribution of the key adhesins that mediate the initial attachment and growth of bacteria to substrates of varying stiffness, at the single-cell level.

- In this project, the student will learn to grow and manipulate bacteria, and measure forces of interactions with substrates using the AFM. The student will acquire and analyze force-extension curves to quantitatively characterize bacterial adhesion.
- The student is required to take WHMIS and Biosafety trainings prior to lab work.
- The student is expected to carry out experiments and analyze data as pre-discussed with the supervisor, meet weekly with the supervisor to track research progress, and write a final thesis report at the end of the project.



References:

- [1] Friedrichs, J, et al. A practical guide to quantify cell adhesion using single-cell force spectroscopy. *Methods*, **2013**, 60, 169-178.
- [2] Sullan RM, et al. Single-cell force spectroscopy of pili-mediated adhesion. *Nanoscale*, **2014**, 6, 1134-43.

Supervisor: Ronald Soong

Co-supervisor (if any): Andre Simpson

Office: SW155B

Sub-discipline:

Laboratory:

Course code: CHMD91

e-mail: ronald.soong@utoronto.ca # of students: 1

Web:

Researching the potential of singlet state NMR for mixture
deconvolution

Singlet state NMR has presented an approach for mixture deconvolution. To achieve singlet state, it requires a particular molecular structure, making this technique suitable for targeted identification. In this research project, the student will conduct a full literature search on the subject and identify molecular structures that can bring about a singlet state. If time permit, simulation will be performed to evaluate under what NMR condition will allow us to achieve single state NMR for mixture deconvolution

- Learning outcomes:
 1. The student will learn to evaluate research literature
 2. The student will learn the basic of quantum mechanics and NMR spectroscopy
- Required training certificates - none
- Our expectations from students:
 1. Work independently
 2. Follow a plan of action that will result in the completion of this project

References:

[1] Journal of Magnetic Resonance 306 (2019) 69–74

Supervisor: Ruby Sullan

Co-supervisor (if any):

Office: EV566

Sub-discipline: Analytical/Biophysical

Laboratory: 5th Floor Labs

Course code: CHMD90/91

e-mail: ruby.sullan@utoronto.ca

of students: 1

Web: <https://www.sullanlab.com/>

Critical Reading of the Literature: Focus on Bacterial Rigidity Sensing

Rigidity sensing—how adherent cells respond to the stiffness of the underlying substrate—is well-known in mammalian cells to be involved in cellular signaling, stem cell differentiation and cancer cell metastasis. It has been shown that contractile forces generated by biological motors (e.g. actin-myosin apparatus) enable rigidity sensing in mammalian cells. In comparison, little is known about the mechanism behind rigidity sensing in bacteria. This Summer Research Project aims to conduct a critical review of the literature on bacterial rigidity sensing. Emphasis will be on the inconsistencies reported on stiffness-dependence bacterial adhesion as a result of the different experimental methods, bacterial strains, stiffness range of surfaces, and surface characterization methods. A central question to answer during the literature review is how to better address these inconsistencies. The student will be exposed to seminal and current works focusing on the relationship between bacterial adhesion and substrate stiffness. Depending on when research operations will resume, this project can continue to hands-on experiments where the student will perform single-cell force measurements to determine the nature of interaction between a suite of bacterial strains and polymeric surfaces with a range of stiffness.

- Learning outcomes
 - Develop familiarity with current and state-of-the art analytical and biophysical techniques used in surface characterization and bacterial adhesion;
 - Critically evaluate experimental data both within a single journal article and in relation to other articles of a similar topic;
 - Communicate a specialized topic—both at its most basic level and broader-theme application;
 - Gain hands-on research experience on the same topic as the critical literature review when research operations will resume.
- Required training certificates
 - WHMIS and Biosafety Training (when lab work will resume)
- Our expectations from students...
 - Meet with supervisor weekly and attend monthly/biweekly group meetings
 - Summarize critical reading of a literature in a written report (as discussed with the research supervisor)

Supervisor: Ruby Sullan

Co-supervisor (if any):

Office: EV566

Sub-discipline: Analytical/Biophysical

Laboratory: 5th Floor Labs

Course code: CHMD90/91

e-mail: ruby.sullan@utoronto.ca

of students: 1

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Critical Reading of the Literature: Biofilm-Nanomaterial Interactions

Treatment of bacterial biofilm-associated infections is challenging, due to their inherent recalcitrance to commonly used antimicrobial agents. This requires the development of new and more effective therapeutic strategies to eliminate biofilm-related infections. The application of nanomaterial-based therapeutic systems is rapidly becoming a plausible alternative to the existing antibiotic-only-based therapy. These nanotechnology-driven applications require understanding of how different types of nanomaterials interact with different components of the biofilm matrix thereby affecting their effectivity in penetrating the biofilm to carry out their therapeutic actions. In this focus literature search, the student will read about and write a review type of article focusing on “*Nanomaterial-based Therapeutics Against Bacterial Biofilms*”. The student will identify antibiofilm strategies where nanomaterials are used (e.g. as drug nanocarriers or nanomaterials that have their own intrinsic antimicrobial activity). Two key areas of focus will be on the synthesis and characterization of the identified nanomaterials as well as the mechanism of its interaction with biofilms.

- Learning outcomes
 - Develop familiarity with current and state-of-the art nanomaterials used as antibiofilm agents and/or drug nanocarriers;
 - Critically evaluate experimental data across relevant and related journal articles;
 - Communicate a specialized topic—both at its most basic level and broader-theme application;
 - Gain hands-on research experience on the same topic as the critical literature review when research operations will resume.
- Required training certificates
 - WHMIS and Biosafety Training (when lab work will resume)
- Our expectations from students...
 - Meet with supervisor weekly and attend monthly/biweekly group meetings
 - Summarize critical reading of a literature in a written report (as discussed with the research supervisor)

Supervisor: Nirusha Thavarajah

Co-supervisor (if any): N/A

Project Discipline: Medicinal Chemistry

Sub-discipline: N/A

Office: EV544

Laboratory: N/A

Course code: CHMD91H3

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of students: 2

Web: N/A

Project Title: A Review on Recent Development of Potential Antiviral Drugs Targeting Severe Acute Respiratory Syndrome (SARS) Corona Virus (SARS-CoV), Middle East Respiratory Syndrome (MERS) Corona Virus (MERS-CoV) and the Novel Coronavirus (COVID-19)

Abstract

Developing new potential anti-viral reagents and obtaining clinical approval is a lengthy process that can take more than a decade. Up to date, there are no effective vaccines or drugs that are clinically approved yet to treat coronavirus, but there are number of potential anti-viral therapeutics that are being explored as viable options. This study will review recent literature for the synthesis and inhibition mechanisms of various classes of antiviral drugs that are being investigated as potential therapeutics for SARS-CoV, MERS-CoV and the novel COVID-19.

Reference

1. Konno, H.; Wakabayashi, M.; Takanuma, D.; Saito, Y.; Akaji, K. *Bioorg. Med. Chem.* **2016**, 24(6), 1241-1254.
2. Ohnishi, K.; Yasunao, H.; Kobayashi, K.; Akaji, K. *Bioorg. Med. Chem.* **2019**, 27(2), 425-435.

Learning outcomes

- Students will learn to do literature search using search engines such as *SciFinder*.
- Students will learn to critically analyze research literature.
- Students will synthesize new knowledge using information in the literature.
- Students will improve their scientific writing skills.
- Students will learn to write a publishable quality scientific article.

Required training certificates: N/A

Our expectations from students:

- Passion for research
- Ability to work independently
- Good time management skills

Supervisor: Prof. Myrna Simpson

Co-supervisor (if any):

Office: SY322

Sub-discipline(s): Environmental, Analytical, Organic

Laboratory: SY315

Course code: CHMB42, CHMB55, CHMC11

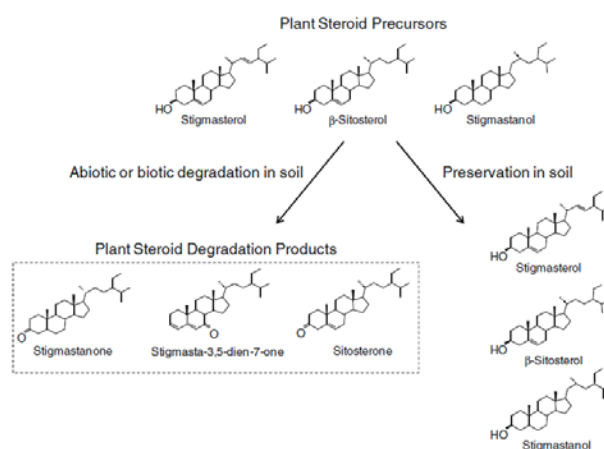
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Antimicrobial properties of plant steroids in soil

Several plant steroids (β -sitosterol, stigmasterol, sitosterone, stigmasta-3,5-dien-7-one, and campesterol) are deposited into soil environments after cell death. Some of these steroids are degraded by bacteria and fungi and some are preserved through binding to the inorganic portion of the soil. Recently, it has been found that when the concentrations of these steroids increase, they exhibit anti-microbial properties and impact the natural process of soil carbon cycling (biogeochemistry) [1]. This project will test how the addition of plant steroids may alter soil biogeochemistry in laboratory incubations.



- **Learning outcomes:** The student will learn about environmental chemistry processes in soil. They will also apply organic chemistry skills to isolate and purify plant-steroids. Laboratory incubations will be monitored using headspace CO_2 analysis and monitor degradation products using GC-MS. The student on this project will be able to apply knowledge in organic, environmental and analytical chemistry to this research.
- **Required training certificates:** EHS005 WHMIS; EHS002 Basic Health and Safety Awareness
- **Student expectations:** The student on this project will be encouraged to attend and participate in Group meetings. The student will meet with the supervisor every 2-3 weeks to discuss project logistics and progress.

References:

[1] Wang, J. et al. *Biogeochemistry* 142, 299–313 (2019)

Supervisor: Prof. Myrna Simpson

Co-supervisor (if any):

Office: SY322

Sub-discipline(s): Environmental, Analytical, Organic

Laboratory: SY315

Course code: CHMB42, CHMB55, CHMC11

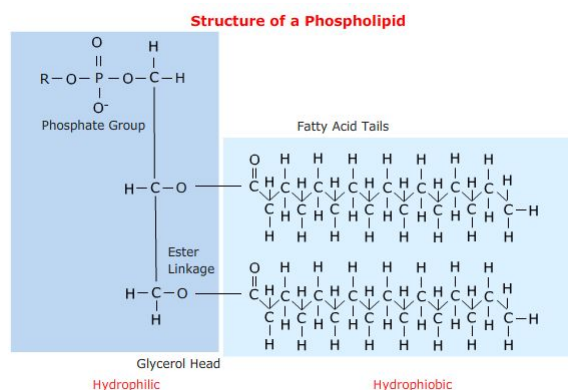
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Can we use ^{31}P NMR to quantify isolated phospholipid fatty acids from soil?

Phospholipid fatty acid (PLFA) profiling is commonly used to measure the total microbial biomass and community structure in soils and sediments. The most common method involves using a Bligh and Dyer extraction followed by several purification and isolation steps to isolate the hydrophobic fatty acid “tails” [1]. Once the extract has been isolated, the lipids are derivatized for GC-MS analysis. The entire process requires 2-3 days of lab work but yields quantitative information about different PLFA types that are indicative of microbial community (actinomycetes, bacteria and fungi). This project will compare quantification of PLFAs using the standard GC-MS method and solution-state ^{31}P NMR of the total lipid extract. The ^{31}P NMR requires less sample preparation steps and could serve as a rapid measure of total microbial biomass. The aim of this project is to compare the two methods and determine the benefits and limitations of each method.



- **Learning outcomes:** The student will learn about organic extraction and purification methods. The student will learn and use GC-MS and NMR for quantification of PLFA fractions. The student on this project will be able to apply knowledge in organic, environmental and analytical chemistry to this research.
- **Required training certificates:** EHS005 WHMIS; EHS002 Basic Health and Safety Awareness
- **Student expectations:** The student on this project will be encouraged to attend and participate in Group meetings. The student will meet with the supervisor every 2-3 weeks to discuss project logistics and progress.

References:

- [1] Frostegård, A. & Bååth, E. *Biol. Fertil. Soils* 22, 59–65 (1996)
- [2] Watts, E. E. & Dean, P. *Can. J. Anal. Sci. Spectrosc.* 47, 127-133 (2002)

Supervisor: O.Voznyy

Office: EV564

Sub-discipline: Electrochemistry

Laboratory: EV306

Course code: CHMD91

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Lithium-ion battery material development

Our group focuses on developing next generation lithium-ion battery materials. This project aims at exploring novel battery electrode materials. The project will mainly involve literature search, material synthesis, coin cell battery assemblies and testing. Students could also be exposed to machine learning and theoretical computations. Students will learn electrochemistry and material science knowledge. Students will work on this project led by a PhD student. This project requires in-person lab experiments.

Qualifications: Completion of CHMA10, CHMA11, and CHMB16 with minimum grade of B+.

Supervisor: O.Voznyy

Office: EV564

Sub-discipline: Electrochemistry

Laboratory: EV306

Course code: CHMD91

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Web: cleanenergy.utoronto.ca

Electrochemical synthesis of ammonia

Our group is interested in electrochemical reduction of nitrogen gas into ammonia in water. The project will mainly involve electrochemistry testing of catalysts, optimizing electrochemical reactors, NMR analysis. Students could also be exposed to theoretical computations. Students will learn electrochemistry, material science, and chemical engineering knowledge. Students will work on this project led by a PhD student. This project requires in-person lab experiments.

Qualifications: Completion of CHMA10, CHMA11, and CHMB16 with minimum grade of B+.

Supervisor: Dr Shadi Dalili

Co-supervisor (if any): Dr Kagan Kerman
Dr Meissam Noroozifar

Office: EV 562

Sub-discipline: Organic/Materials

Laboratory: EV 124

Course code: CHMD90Y

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of students: 1-2

Application of COFs and MOFs in solar cells

The main goal of this project is development of covalent organic frameworks (COFs) and/or metal organic frameworks (MOFs) as a new generation of materials for solar cells (SC). One of the major issues in current solar cells is that they are not stable with a light simulator (SUN), due to unstable sensitizers, whose role is to allow for absorption of the light and injection of photoexcited electrons into the conduction band of TiO₂ as semiconductor. Generally, the sensitizers decompose with the SUN.

COFs and MOFs composed of a high number of C-C, C-O, C-H, and M-O bonds have shown to create high thermal stability between 300-500°C. Along with this high thermal stability, high chemical stability, tunability in pore or channel architecture, and the ability to change chemical properties after synthesis via post-synthetic techniques are the most attractive properties in these materials.

Our hypothesis is that based on this heterojunction between MOF with the TiO₂ and other elements in SC, the efficiency of SC can be increased.

The successful candidate(s) for the project will conduct a comprehensive literature research on the different types, applications and syntheses of COFs and MOFs and use this information to propose and design novel COFs and MOFs that could show high stability with high molar absorptivity by varying the different organic moieties in the structures. The 2nd stage of the project will be the synthesis and characterization of the proposed structure(s) and subsequent building of the solar cells and testing of compounds in the SC in Dr. Kerman's lab under co-supervision and conceptualization by Dr. Meissam Noroozifar.

Supervisor: Dr Shadi Dalili

Co-supervisor (if any): Dr Kagan Kerman
Dr Meissam Noroozifar

Office: EV 562

Sub-discipline: Organic/Materials

Laboratory: EV 124

Course code: CHMD90Y

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of students: 1-2

Development of novel Hole Transport Materials (HTMs) for application in Perovskite solar cells

Perovskite solar cells (PSCs) have witnessed dramatic developments with the record power conversion efficiency (PCE) exceeding 25% within a single decade. One bottleneck for the commercialization of PSCs is the lack of stability due to the commonly used hole transport materials (HTMs) with dopants.¹

The main goal of this project is to review the recent progress in dopant-free HTMs, including organic small molecules, polymers, organometallic compounds, and inorganic materials, and propose detailed solutions for making dopant-free HTMs more efficient, stable, and cost effective.

The successful candidate(s) for the project will conduct a comprehensive literature research on the different types, applications and syntheses of current dopant-free HTMs and use this information to propose and design novel HTMs that could show high stability, efficacy, and applicability in Perovskite solar cells. The 2nd stage of the project will be the synthesis and characterization of the proposed structure(s) and subsequent building of the solar cells and testing of synthesized HTMs in the SC in Dr. Kerman's lab under co-supervision and conceptualization by Dr. Meissam Noroozifar.

¹ Toward ideal hole transport materials: a review on recent progress in dopant-free hole transport materials for fabricating efficient and stable perovskite solar cells; Xinxing Yin, Zhaoning Song, Zaifang Li, and Weihua Tang; *Energy Environ. Sci.*, **2020**, *13*, 4057

Supervisor: Dr Shadi Dalili

Co-supervisor (if any):

Office: EV 562

Sub-discipline: Organic/Bio-organic

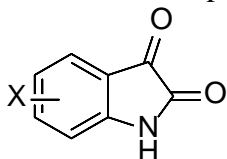
Laboratory:

Course code: CHMD90Y/CHMD91H

e-mail: sdalili@utsc.utoronto.ca # of students: 1

Synthesis and Biological Activity of Isatin Derivatives

Isatin (1H-indole-2,3-dione) is one of the most favorable type of heterocyclic systems that possesses many interesting biological activities and well-tolerated in humans. Isatin and its derivatives such as Schiff bases, can be used as precursors for drug synthesis. Reactivity of Isatin towards different electrophiles and nucleophiles, as well as the firmness of its indole ring, has generated considerable attention among medicinal chemists, in order to create many pharmacophore moieties to obtain novel bioactive compounds.



X= H, F, Cl, Br.

Isatin and substituted Isatin

Due to the great potential of Schiff bases of Isatin as anti-cancer agents, in this collaborative project, we plan to synthesize some new Schiff bases of N-substituted Isatin and evaluate their anticancer activities. These compounds will be synthesized in a two-step reaction, including benzylation (alkylation) and Schiff bases production. The final products will be identified and characterized by various spectroscopic methods such as IR, Mass Spectrometry and NMR. We will then investigate the anti-oxidant properties and cytotoxic activities of these compounds in collaboration with Dr Kagan Kerman, as well as the anti-proliferative effect of these synthetic compounds against different tumor cell lines in order to publish original research in high impact journals.

The project will commence with relevant literature research and writing of introduction sections for the manuscripts to be published, followed by synthesis work in the lab of the various derivatives.

This project may be extended into the Winter 2021 semester to allow sufficient time in the lab for synthesis of desired compounds, as a CHMD90Y project. However, it can also be conducted as a CHMD91H literature research project along with research proposal for lab synthesis.