CHEM4710

Honours Project

in

Chemistry or Biochemistry

2024/2025 Projects

University of Manitoba

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1. WELCOME

Welcome to the 'Honours Project in Chemistry or Biochemistry' (CHEM4710) for the 2024/25 academic year. The 'Honours Project in Chemistry or Biochemistry' is a research project based course providing undergraduate chemistry and biochemistry students with the opportunity to conduct original research as part of an active research group. The research project extends over a duration of 2 consecutive terms (Sep. 2024 – Apr. 2025). Students can request projects based on the list of projects provided in this booklet. Each project can only have 1 CHEM4710 student. We will ensure that the project assignments are fair to all students. Project selections will be carried out at the beginning of August 2024.

Throughout the research projects students will receive guidance and support from their research advisors and other research group members. Notably research environments are very diverse in the Department of Chemistry and naturally individual research groups may operate differently and have varying foci. Specifics need to be discussed with the project advisors. The Department of Chemistry at the University of Manitoba is a medium size department and is well situated within the top 15 Canadian Universities (U15). In general the research groups in the Department of Chemistry are highly competitive, recognized in their respective fields and contribute to the large fields of chemistry and biochemistry. The experimental and theoretical opportunities offered in the Department of Chemistry are excellent with well equipped laboratories, state-of-the art instrumentation and outstanding expertise. The majority of the research is being conducted in the Parker Building Notably many groups collaborate with other departments, faculties/schools and institutes within the University of Manitoba. The majority of research groups maintain national and international collaborations and are part of large scale facilities such as national laboratories and institutes all around the world.

It should be noted that biochemistry students can choose to take MBIO4530 instead of CHEM4710 for credit for their program.

I sincerely hope that you will explore the opportunities accessible in the Department of Chemistry by looking at the project descriptions in this booklet and that you will take the opportunity to meet with faculty members and discuss their projects within the framework of CHEM4710.

I am looking forward to a research-filled year of CHEM4710 projects for 2024/25.

Dr. Mario Bieringer

Course coordinator for CHEM4710 2024/25

2. INTRODUCTORY COMMENTS:

Students interested in taking CHEM4710 should look at all offered projects provided in this booklet and need to contact project supervisors and discuss projects listed in this booklet. During those meetings the nature of the projects should be discussed and expectations should be made clear. Please note that project advisors are happy to meet with you to discuss their research projects. Students are expected to meet with at least 3 faculty members and are required to complete the 'Student – Faculty Interviews' page (Appendix A). Please prioritize your project choices on the attached 'Student Project Choices' page (Appendix- B). A minimum of 3 choices should be submitted and comments can be added in the provided comment field. In order to be considered for the entire set of advertised projects you are asked to submit the 'Student – Faculty Interviews' page and 'Student Project Choices' page with your project choices to Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca) by July 29th, 2024. Matching of students with research projects will only occur after July 29th, 2024. Students can submit their project choices after that date as well, however the number of available projects might be limited by then. Students will be informed about their projects by August 6th, 2024.
The research projects will start during the first week of the 2024 Fall term. For each project the student and project advisor must submit a completed and signed 'Student – Advisor Agreement' (Appendix-C) no later than September 13th, 2024. Please note that this agreement clearly describes the obligations of both parties. In addition to the research conducted in the individual research groups there will be mandatory class meetings for CHEM4710. Those meetings will cover general topics relevant to your research activities and will provide you with important skills related to the project course. The class meetings will also help in getting to know all research project students. The dates for the class meetings are tentative. Students should reserve the Friday time slot from 1:30 pm till 2:20 pm for CHEM4710 meetings for the Fall 2024 and Winter 2025 terms. It is important for students to communicate regularly with their project advisors, share information about research progress, research needs, administrative needs and talk about upcoming deadlines.

The progress report is due on November 8th, 2024. The expectations for the progress report are clearly stated in the course syllabus. The research projects should be concluded by the end of the 2025 Winter term. On Saturday March 29th, 2025 each student will present a 15 minute talk followed by 5 minutes of questions during a conference style presentation day. Students and advisors should reserve this day for the presentations. This will be a public event and faculty members, students, friends, family and other guests are welcome to attend. The final written reports will be due on April 10th, 2025. The final report will be graded by an expert reader who is familiar with the research subdiscipline and a non-expert reader whose research is in a different subdiscipline.

3. IMPORTANT DATES & DEADLINES

Jul. 29th, 2024	Students submit project choices to the course coordinator
Aug. 6th, 2024	Students receive project assignments
Sep. 4th, 2024	Students begin research projects (first day of classes)
Sep. 6th, 2024	Class meeting #1 - Orientation meeting (all students and supervisors)
Sep. 20th, 2024	Signed contracts (Student – Advisor Agreement) DUE
Sep. 20th, 2024	Class meeting #2 (Library resources and literature search)
Oct. 4th, 2024	Class meeting #3 (Academic integrity)
Oct. 18th, 2024	Class meeting #4 (Report writing and proposal development)
Nov. 1st, 2024	Class meeting #5 (3 minute project presentations)
Nov. 8th, 2024	Written progress report DUE
Nov. 19th, 2024	Voluntary Withdrawal DEADLINE (UofM)
Nov. 22nd, 2024	Class meeting #6 (Career choices in chemistry and biochemistry)
Dec. 6th, 2024	Class meeting #7 (Academic writing & peer review process)
Jan. 10th, 2025	Class meeting #8
Feb. 24th, 2025	Class meeting #9
Jan. 31st, 2025	Last day for students to meet with course coordinator for proposal discussion
Feb. 7th, 2025	Student proposals DUE
Feb. 7th, 2025	Class meeting #10 (Effective oral presentations)
Feb. 14th, 2025	Student evaluations of proposals DUE
Feb. 28th, 2025	Class meeting #11
Mar. 14th, 2025	Class meeting #12
Mar. 28th, 2025	Class meeting #13
Mar. 25th, 2025	Title and abstracts for oral presentations DUE
Mar. 29th, 2025	Oral research project presentation day
Apr. 10th, 2025	Final written reports DUE

4. DRAFT COURSE SYLLABUS

GENERAL COURSE DESCRIPTION:

CHEM4710 is a 6 credit hour research project course spanning over the Fall 2024 and Winter 2025 terms. Each student will carry out research as a member of a research group in the Department of Chemistry. Students in CHEM4710 are expected to begin work on their research project at the beginning of September 2024 and to maintain a steady level of work during the entire academic year.

All available course projects will be made available to all students interested in or considering in taking CHEM4710 in Fall 2024/Winter 2025. Each project will consist of a brief 1 page description. Students are encouraged to read all projects and arrange appointments with supervisors for a brief interview/discussion. Each student needs to meet with at least 3 potential supervisors. Following those meetings students should submit their preferred project choices to the course coordinator in order of preference (e.g. 1st choice: "The investigation of ….", 2nd choice: "Synthesis of …", etc.). Project matching will commence after Jul. 29th, 2024 and the project assignments will be e-mailed to the students and supervisors on August 6th, 2024.

Throughout the project students are expected to consult regularly with their advising professor to ensure that adequate progress is being made. Each student in CHEM4710 is expected to conform to university standards of laboratory safety at all times and will also meet the standards of the research group that they are working in with regard to experimental procedures, notebook keeping, and general laboratory behavior.

The role of the student is to be an active and productive member of the hosting research group. CHEM4710 students will work on their own specific projects that are assigned. However, this project is likely integrated into the larger research program underway in the research group. Therefore, communication with group members and the research advisor is extremely important. The CHEM4710 project is an excellent opportunity to participate in the "life" of the research group and to learn from the senior members. Your active participation in the group as part of the CHEM4710 experience can also give you a good impression of what graduate studies would be like. Good performance in the group may earn you a positive reference from your advisor for any future applications for graduate studies, other degrees or for entry into the workforce.

The role of your advisor is to help guide your entry into the world of research. This quite often is a markedly different experience than what you have experienced in typical teaching laboratories. The transition into independent research can be challenging in some cases. The role of the advisor is to help you, point you at relevant literature, describe the opportunities and pitfalls, while at the same time avoiding guiding you in minute detail. The success of your research project lies with your ability to work in the research lab in a self-motivated manner and to develop a measure of independence in your abilities. Although your advisor is available to provide guidance on the preparation of your research proposal, reports, and presentations, however the responsibility for the completeness of these course requirements rests solely with the student.

CHEM4710 projects provide the opportunity to develop practical lab skills beyond those that are usually taught in a 1st, 2nd or 3rd year laboratory course. The CHEM4710 course also provides the opportunity to develop other essential skills such as self-motivation and time management that allow you to be organized in your research. You will also be required to describe your results in a format that is more than a simple 'lab report' in both the written and oral presentation. A major part of the evaluation of your performance is on how well you develop these skills and not necessarily on the perceived success of your project. One meaningful result, generated in September, poorly reported on and described in a rambling talk will not as high as a series of carefully recorded experiments repeated several times and described in detail that nonetheless did not generated the 'expected' results etc.

I) INSTRUCTOR INFORMATION:

Course Coordinator:

Name: Dr. Mario Bieringer

Office: 520c Parker Building

E-mail: Mario.Bieringer@UManitoba.ca

Phone: (204) 474 6258

II) EVALUATION:

3 minute presentation	3 %
Written Progress Report	14 %
Proposal	8 %
Oral Presentation	20 %
Research Effort (Evaluated by the research advisor(s))	20 %
Written Final Report (Evaluated by 2 readers)	35 %

Final numerical scores will be converted to letter grades. As this is a senior level course, the marking scale will assume that F = less than 50%. Other scores will be scaled appropriately between D and A+ as described below.

Percentage Score	Letter Grade	Grade Point Value
90.0 -100.0	A+	4.5
80.0 - 89.9	A	4.0
75.0 - 79.9	B+	3.5
70.0 - 74.9	B	3.0
65.0 - 69.9	C+	2.5
55.0 - 64.9	C	2.0
50.0 - 54.9	D	1.0
0.0 - 49.9	F	0.0

III) COURSE PARTICIPATION:

- Students are encouraged to attend the Departmental Seminars.
- Attendance of all Friday CHEM4710 class meetings (listed in the table below) is mandatory.

Date	Time	Location	CHEM4710 Class Meetings	Presenters
Sep. 6th, 2024	1:30–2:20pm	t.b.d.	Orientation Meeting	Mario Bieringer
Sep. 20th, 2024	1:30-2:20pm	t.b.d.	Library and literature searches	Marie Spears
Oct. 4th, 2024	1:30–2:20pm	t.b.d.	Academic Integrity	t.b.d.
Oct. 18th, 2024	1:30–2:20pm	t.b.d.	Report and proposal writing	Mario Bieringer
Nov. 1st, 2024	1:30–3:20pm	t.b.d.	3 Minute Presentations	Students
Nov. 22nd, 2024	1:30–2:20pm	t.b.d.	Career choices	Mario Bieringer
Dec. 6th, 2024	1:30–2:20pm	t.b.d.	Academic writing & peer review	Mario Bieringer
Jan. 10th, 2025	1:30–2:20pm	t.b.d.	t.b.d.	t.b.d.
Jan. 24th, 2025	1:30–2:20pm	t.b.d.	t.b.d.	t.b.d.
Feb . 7th, 2025	1:30–2:20pm	t.b.d.	Effective oral presentations	Mario Bieringer
Feb. 28th, 2025	1:30–2:20pm	t.b.d.	t.b.d.	t.b.d.
Mar. 14th, 2025	1:30–2:20pm	t.b.d.	t.b.d.	t.b.d.
Mar. 28th, 2025	1:30–2:20pm	t.b.d.	t.b.d.	t.b.d.

IV) IMPORTANT DATES:

The dates below are fixed and no extensions are possible.

Date	Milestone
Jul. 29th, 2024 (Monday)	Students submit project preferences to the course coordinator
Aug. 6st, 2024 (Tuesday)	Students receive project assignments
Sep. 20th, 2024 (Friday)	Signed research contract due
Nov. 8th, 2024 (Friday)	Written progress report due
Jan. 31st, 2025 (Friday)	Last day for students to meet course coordinator for proposal discussion
Feb. 7th, 2025 (Friday)	Proposals due
Feb. 14th, 2025 (Friday)	Student evaluations of proposals due

Mar. 25th, 2025 (Tuesday)	Title and abstract for oral presentations due
Mar. 29rd, 2025 (Saturday)	Oral presentation day
Apr. 10th, 2025 (Thursday)	Written final report due

V) DESCRIPTIONS OF COURSE COMPONENTS:

- Project Descriptions
  Students should read all project descriptions and arrange for a minimum of 3 meetings with potential project supervisors. Supervisors must be full time faculty members in the Department of Chemistry. Please note that potential supervisors cannot promise projects to students.

- Project Preferences
  Due Monday July 29th, 2024 for the first project selection round. Students should submit their project preferences by that date by e-mail to the course coordinator (Mario.Bieringer@UManitoba.ca). The forms for this submission are part of the project description booklet. Students submitting their project requests after July 29th, 2024 may only be able to choose from a smaller (i.e. remaining) set of available projects.

- Project Assignments – Available Tuesday August 6th, 2024
  Students and supervisors will be informed regarding their projects on August 6th, 2024. It should be noted that every effort will be made to match students with their highest priority choices. However, this will not always be possible because multiple students may apply for the same project. Students applying for projects after July 29th, 2024 may do this up to the late registration deadline, however it is strongly encouraged that students start meeting with supervisors early on and submit their preferences as early as possible.

- Written Progress Report – Due Friday November 8th, 2024 (submit to Mario Bieringer)
  The Progress Report will be handed in to the course coordinator by e-mail (Mario.Bieringer@UManitoba.ca) for marking.

  The report should consist of:

  - a description of the goal(s) of the research project,
  - a detailed survey of the relevant literature that puts the project in context,
  - a description of the planned methods for the research project,
  - a summary of your research results during the Fall term including experimental data.

  The progress report should be about 2000 – 3000 words in length with double-spaced pages and will include any relevant figures and references (which are not included in the word count). It should conform to one of the formats described below for the Final Report. Students should have their research supervisor review and approve their report before handing it in to the course coordinator. It is important that the report makes the project clear to a scientifically literate but non-expert reader.
  The Progress Report is a crucial document that makes sure that projects are progressing, that there are no misunderstandings in terms of expectations and that the relevant literature has been digested. The graded progress reports will be returned to the students with comments and suggestions. The comments will be important for preparing the final report and for the oral presentation. It is well worth the effort to ensure that the progress report is as complete as possible as this effort will pay off at the end of the course. Electronic progress reports must be received by e-mail by the end of day on Nov. 8th, 2024 to be considered for credit in the course.

- Proposal - Due Wednesday February 7th, 2025
  The proposal is a 2 to 3 page document with additional figures and references based on the students research project. The purpose of the proposal is that based on the critical evaluation of the students research (results, difficulties, challenges etc.) a concise request for follow up research will be written. Students are not supposed to propose new research, instead the request should enable the student to further or complete their current research. The following cases highlight possible proposal requests:

  - If a student has experienced challenges that cannot be addressed in the current research group, the student may choose to write a proposal for access to an external research facility or a request for a collaboration.
  - A proposal could also focus on obtaining specific materials (e.g. isotopes, starting materials, experimental probes).
  - Alternatively, the proposal may focus on developing the current emphasis of the project towards a new direction (but not a new project)
  - etc.

  Proposals should be discussed with and approved by the course coordinator no later than Jan 31st, 2025. Every student will have to e-mail a brief outline of the proposal to the course coordinator before that meeting, a couple of sentences are sufficient. The course coordinator needs to be given the chance to at least identify the overall direction of the proposal before meeting with the student. The coordinator will comment and advise on the proposal during the meeting.

  The final proposal will be peer reviewed by 2 CHEM4710 students and the course coordinator. The students need to submit their evaluations to the course coordinator by February 14th, 2025. Students will receive grades for their evaluations. The total proposal mark will be based on the quality of the student's proposal (graded by 2 student and the course coordinator) and the student's evaluations of other proposals..

- Title and Abstract for oral presentations - Due Tuesday March 25th, 2025
  The Title and Abstract must be e-mailed to Mario Bieringer (Mario.Bieringer@UManitoba.ca) by Tuesday March 25th, 2025. It is important to meet this deadline in order to create a presentation schedule on time for the oral presentation day.

- Oral Presentations - Saturday March 29th, 2025
  You will be required to give a 15 minute oral presentation summarizing your research project. The presentation will be followed by 5 minutes for questions. The presentations will be moderated and the time limits will be strictly followed. An oral presentation normally consists of an introduction, a brief description of relevant methods, results and discussion, and conclusions; the last slide is typically an acknowledgment of the advisor and assistance provided by others during the project as well as financial support. The oral presentation should not be generic, because of the limited time the introduction needs to be very targeted towards the project and any data presented need to be prepared in a conscientious manner. It is essential that students prepare and practice their presentations to effectively communicate their project within these time limits. There will be a scoring penalty for exceeding the 15 minute time limit on the presentation.

  Please note that the final presentations are open to all members of the university community as well as the public and will be advertised on campus. Partners, family members and friends are particularly welcome to attend. Recording of any of the presentations will NOT be permitted.

  The use of PowerPoint (or equivalent software) is the standard for scientific presentations. You should plan to give your oral presentation using the computer that is provided in the room – or with your own laptop if you choose.

  This is a full day public event resembling a small conference. The audience usually consist of faculty members, research associates, postdocs, graduate students, undergraduate students and visitors such

as friends and family members. All members of the audience will be allowed to ask questions. All CHEM4710 students are required to grade all (except their own) presentations, in addition all other audience members are encouraged to grade the presentations.

The presentation day is really a celebration of accomplished research and recognizing growth as researchers.

- Final Report - Due Thursday April 10th, 2025 (12 days after the oral presentations)

  The final report is a major part of the evaluation for the project course. It will be marked by two readers. One reader will be close to your research sub-discipline, the second reader will be a faculty member from the Department of Chemistry who is not an expert in your sub-discipline.

  You need to submit the final report as a properly formatted PDF document to the course coordinator (Mario.Bieringer@UManitoba.ca). The course coordinator will distribute the reports to the two readers.

  Each reader will grade your report, both reviews together will be worth 35% of the course grade. It must be emphasized that the report has to be comprehensible to the general scientifically literate reader, and this will be taken into account when marking it. The report must show that you understand the context of the project as well as the actual experiments that you have done. The typical length for the final report is 6000 – 8000 words with double-spaced pages and including figures and references (which are not included in the word count). The exact length will depend on the style of reporting that is specific to the sub-discipline that your project falls in.

  The final report must be a formal piece of scientific writing, with Introduction, Results, Discussion, Conclusion and Experimental (Methods) sections. You may find it more effective if the Results and Discussion sections are combined. The report should also include the relevant figures and references as needed to make the report complete and clear. It should follow the style conventions of an appropriate scientific journal, the American Chemical Society (ACS) journals provide good templates to follow. Stylistic rules are found on journal Web pages and students are encouraged to consult the journal (i.e. J. Am. Chem. Soc.; J. Org. Chem. or J. Phys. Chem., Biochemistry) most appropriate to their project. Another useful resource is the ACS Style Guide which offers useful information on formatting and referencing. Consult your advisor before beginning to write, to determine an appropriate approach. Students should have a draft of the report completed by early-March. Advisors are urged to provide constructive comments on their students' draft reports before the final version is submitted.

  Written reports should be reasonably free of typographical errors and be checked thoroughly for spelling and grammar. Frequent spelling or grammatical errors detract from the readability of your proposal, report or presentation, generate an impression of sloppiness with the audience, and will often result in a lower grade. The same applies to inconsistent formatting of text and figures in the report and references. Therefore, you are strongly advised to use the spelling and grammar checking functions on your word processing software. In addition, you will find the formatting and document handling features of the word processing software very useful. You should consider asking other members of your research group or another student in the project course to help proofread your documents. Your supervisor will be very willing to provide feedback on the content of your report, and this will be more meaningful on a report free of errors.

  The target audience, for your proposal, oral presentation and formal reports, is a student at approximately your stage in the Chemistry or Biochemistry program who may not be familiar with the specifics of your research project. The use of acronyms and shorthand notations should be kept to a minimum but if used those need to be fully explained. The formal report should attempt to describe in as much detail as possible all of the work you have done during the course of the project.

However, in your oral presentation - where you have limited time - you may wish to provide a summary of the most significant results that you generated.

VI) ADDITIONAL INFORMATION:

Conference Opportunities

- The 2025 Western Canadian Undergraduate Chemistry Conference (WCUCC – 2025)
  It is highly recommended for all CHEM4710 students to consider presenting their research at the 2025 'Western Canadian Undergraduate Chemistry Conference' (WCUCC). This annual conference usually takes place in May in one of the universities west of Ontario. Date and place will be communicated at a later point in time. The format of oral presentations is identical to that used in CHEM4710, so you will already have a talk prepared by the time the course is complete. It is a superb opportunity for you to start some professional networking, and there are cash prizes for outstanding presentations. Interested students need to pre-register in January or February for this conference. There are some travel funds available for students (or groups of students) that intend to present at this conference.

- Canadian Chemistry Conference and Exhibition (CCCE-2025)
  The Canadian Chemistry Conference and Exhibition 2025 (CCCE-2025) is the national conference for chemists in Canada with up to 2000 delegates from all over Canada and a significant number of international speakers. The conference will be held in Ottawa from June 15th till June 19th, 2025 and will provide an excellent opportunity to highlight your research and to network with globally leading researchers. CHEM4710 students are encouraged to present their research at the CCCE-2025. The CHEM4710 project provides an excellent base for presenting a poster at that event. Note that conference registration is expected between the 1st week of January and mid February 2025.

VII) USE OF ARTIFICIAL INTELLIGENCE:

All submissions for CHEM4710 need to be generated by the student. The use of Artificial Intelligence (AI) for generating documents is not permitted. It should be noted that effective tools for the identification of AI generated documents exist.

Be aware that submission of your research results to AI make those data semi-accessible to others, because your submission will be part of the learning process of the AI software. This can have significant impacts on intellectual property (IP) rights.

VIII) ACADEMIC INTEGRITY POLICIES:

Academic Dishonesty:

The University of Manitoba treats plagiarism and cheating as serious academic offenses.

- The complete documentation regarding cheating, plagiarism and fraud be accessed in the calendar at:
  http://umanitoba.ca/student/resource/student_advocacy/cheating_plagiarism_fraud.html
- Additional documentation is available on the Faculty of Science website
  https://sci.umanitoba.ca/statement-on-academic-dishonesty/

END OF SYLLABUS

5. PROJECTS

The following projects are being offered under the course number CHEM4710.

Project #1:
Designing New Preparative Routes for Next Generation Thermal Expansion Materials

Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca, (204) 474 6258)

INTRODUCTION:

Solid state materials are dominating the majority of communication, energy, sensing, electronic and optical technologies. Solid state oxides are particularly enticing due to their large density of functional metal cations and their diverse structures. Surprisingly the formation pathways and mechanisms are only very poorly understood. In order to advance materials chemistry such as switching from environmentally concerning and toxic materials to the preparation of high-performance benign materials the synthesis of those materials need to be understood. Thermal expansion describes the volume change of a material as a function of temperature. While the majority of structures expand upon heating there are also negative thermal expansion materials known that undergo volume contraction upon heating. Particularly important are isotropic materials that show identical properties along all 3 principal directions. A key structural component for negative thermal expansion materials is a network of corner connected polyhedra. ZrW_2O_8 is a good structural example with corner connected ZrO_6 octahedra and WO_4 tetrahedra acting as 3-dimensional hinges permitting volume reduction upon heating.[1]

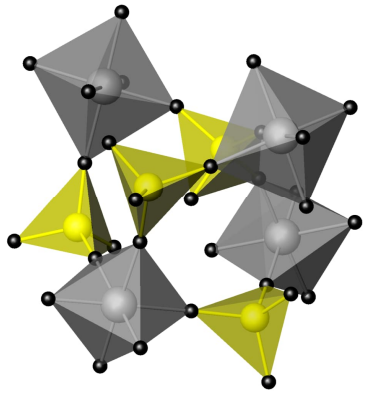

Figure 1: *Fragment of the ZrW_2O_8 structure. Yellow = W^{6+}, grey = Zr^{4+} and black = O^{2-}. Note that all polyhedra are corner connected.*

PROJECT:

In this project novel materials with corner sharing octahedra based on the ReO_3 structure will be developed. Notable $CaSnF_6$ is a superstructure of the ReO_3 structure type. The structure of $CaSnF_6$ is shown in figure 2 forming a network of corner sharing octahedra. Using fluoride anions permits to use an average cation oxidation state of 3+, thus permitting the combination 2+ and 4+ cations and in case of transition metals those can oxidation states can be fine tuned using redox chemistry. It is proposed to form $A^{4+}B^{2+}F_6$ and $A^{3+}B^{3+}F_6$. The structures of those new compounds will be solved using powder X-ray diffraction and thermal expansion measurements will be conducted using high-temperature *in-situ* powder X-ray diffraction. The structures can be fine tuned via redox chemistry generating systems such as $A^{4+}B^{2+}{}_{1-x/2}B^{3+}{}_{x/2}F_{6-x}O_x$. This project will provide students with a strong background in materials chemistry coupled with materials characterization.

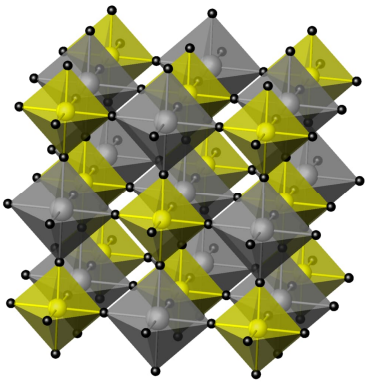

Figure 2: *Cubic $CaSnF_6$ structure. Yellow = Sn^{4+}, grey = Ca^{2+} and black = F^-. Note that all polyhedra are corner connected.*

References:

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[2] Q. Gao et al. Nano Research, 2023, 16(4): 5964−5972

Project #2:
Preparation and Reactivity of ZrO_2 based Oxide Ion Conducting Materials for Solid Oxide Fuel Cell Applications

Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca, (204) 474 6258)

INTRODUCTION:

Solid Oxide Fuel Cells (SOFCs) are highly efficient and fuel tolerant devices for the conversion of chemical energy directly to electrical energy. Fuel cells are compact and virtually maintenance free if exclusively designed with solid state materials. Currently the major drawback of SOFCs is the high operating temperature of almost 1000°C. In an effort to lower the operating temperature of SOFCs oxide defect structures based on ZrO_2 are being synthesized and the formation of the oxide defects are investigated systematically, fig. 1.

PROJECT:

Yttria stabilized zirconia, $Zr_{1-x}Y_xO_{(2-x/2)}\square_{x/2}$ (where $\square$ denotes oxide defects, i.e. missing O^{2-} anions) are cubic fluorite structures with randomized oxide defects.
In order to investigate the creation and annihilation of these oxide defects it is proposed to replace Y^{3+} with $Pr^{3+/4+}$ cations. With the addition of Pr^{4+} to ZrO_2 a redox active cation allows the reversible removal of oxide anions during reduction and repopulation of the oxide defects with actual oxide ions during oxidation. In this project $Zr_{1-x}Pr_xO_2$ will be prepared using high temperature reactions. The reversible oxide uptake and removal will be investigated using in-situ powder X-ray diffraction experiments and thermogravimetric analysis in order to determine structural details and oxygen stoichiometries as a function of reaction conditions. Ion conductivities will be measured for this system under redox conditions. Students carrying out this project should be familiar with inorganic chemistry and willing to learn structure determination techniques for crystalline solids and be interested in characterization of physical properties. Laboratory skills and data analysis will be one of the many potential learning outcomes of this project.

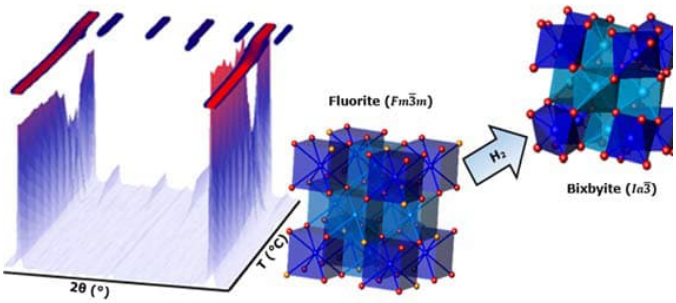

Figure 1: Real time *in-situ* X-ray diffraction experiments illustrating the selected oxide removal from the disordered fluorite structure (right structural diagram) during reduction of $Y_{(1-x)}Pr_xO_{3.5}$.

References:

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Project #3:
Preparation of Novel Quantum Magnets

Dr. Mario Bieringer (Mario.Bieringer@UManitoba.ca, (204) 474 6258)

INTRODUCTION:

Materials science is largely based on solid state materials. Among magnetic materials particularly interesting are examples that do not show classical long range magnetic ordering at low temperatures. Magnetic ordering can be manipulated by disorder and competing magnetic exchange paths. E.g. a triangle of paramagnetic cations (e.g. V^{4+} or Ti^{3+}) with antiferromagnetic coupling results in magnetic frustration, i.e. at least one of the magnetic moments is not able to satisfy all interactions simultaneously, see figure 1. For large magnetic moments a 120° compromise structure may be observed. In contrast small magnetic moments (e.g. d^1 ➔ S=1/2) may form exotic magnetic ground states enhancing our fundamental understanding of magnetic interactions. This concept can be further expanded to tetrahedral motifs, see fig. 2. Quantum magnets fall into this category and are under intense investigation for quantum computing applications.

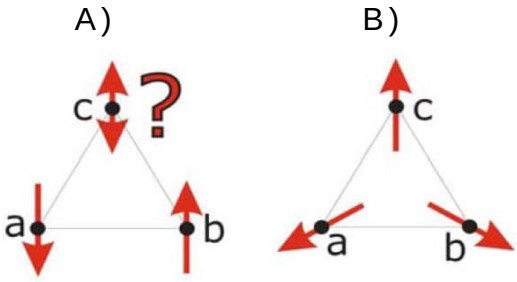

Figure 1: *A) Geometric magnetic frustration. 3 spins on a triangular lattice cannot align antiparallely with respect to each other. B) 120° magnetic structure for*

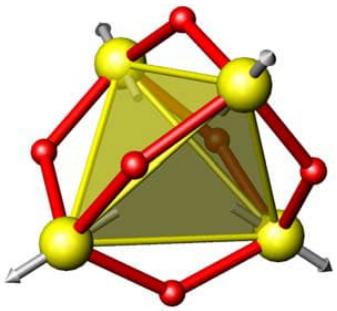

Figure 2: *Tetrahedral spin arrangement on metals (yellow) with oxide (red) bridges responsible for magnetic exchange.*

PROJECT:

In this project novel materials with triangular and tetrahedral magnetic lattices will be synthesized and the transition metal oxidation states will be fine-tuned in order to realize quantum behaviour. The work will be based on ABO_3 and ABO_4 structures where A is a diamagnetic cation (Ca, Sr, La, Y, Lu etc.) and B is a redox active cation such as Ti, V, Cr, Mn or Fe etc. Notably the ABO_3 and ABO_4 samples are chosen in order to further reduce or oxidize the parent compounds under mild conditions (use of buffer gases and solid state hydrides in particular). This project consists of a synthetic component, a structure determination (diffraction) part in order to establish the newly generated phases and advanced physical property measurements. The advanced characterization will potentially include magnetic measurements, neutron scattering (NPD), X-ray photoelectron spectroscopy (XPS) and related EXAFS and XANES experiments. This project will provide students with a strong background in materials chemistry coupled with materials characterization.

References:

[1] S. Nishimoto et al., Nature Communications. (2016) 7, 10273
[2] B. Hernden, J.A. Lussier, M. Bieringer, Inorg. Chem. (2015), 54, 4249−4256
[3] D. Vrublevskiy et al., Inorg. Chem. (2021) 60, 872-882

Project #4:
Adaptive Laboratory Evolution of *Escherichia coli*:
Synthetic Life Microbes that Thrive on Plastic or Synthetic Substances

Dr. Nediljko Budisa (nediljko.budisa@umanitoba.ca, (204) 474 9178)

INTRODUCTION:

We aim to create synthetic cells through top-down synthetic biology, focusing on engineering *Escherichia coli* to metabolically adapt to synthetic amino acids and materials like plastics as their sole carbon source. These biosafe cells will produce protein-based biomaterials crucial for tissue engineering, materials science, and environmental remediation. Our research environment prioritizes student learning in synthetic biology and organism-directed evolution.

PROJECT:

Our first experiment involves performing adaptive laboratory evolution (ALE) of *E. coli* cells in a medium containing fluorinated amino acids or plastics such as PET as the sole carbon source. Students will participate in the development of experiments with evolving microbial cultures with synthetic substances. The ALE experiments will focus on the creation of auxotrophic *E. coli* strains capable of metabolising halogenated amino acids or plastic. In ALE, several lines (at least 4) are used to distinguish adaptive mutations from hitchhiker mutations, supported by control experiments. Analysing the ALE process will provide insights into cellular functions, genetics, proteomics, and morphology, thus advancing synthetic biology for the development of innovative technologies.

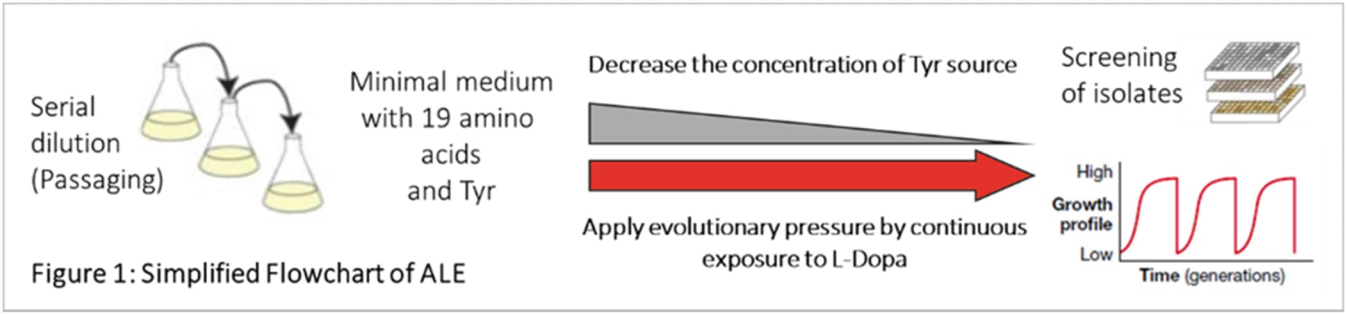

Figure 1: Simplified Flowchart of ALE

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2. I Tolle, et al. & AC Gerstein, N Budisa (2023) Evolving a mitigation of the stress response pathway to change the basic chemistry of life. *Front. Synth. Biol*. 1:1248065 (doi: 10.3389/fsybi.2023.1248065).

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Project #5:
Expanding the Genetic Code by Directed Enzyme Evolution

Dr. Nediljko Budisa (nediljko.budisa@umanitoba.ca, (204) 474 9178)

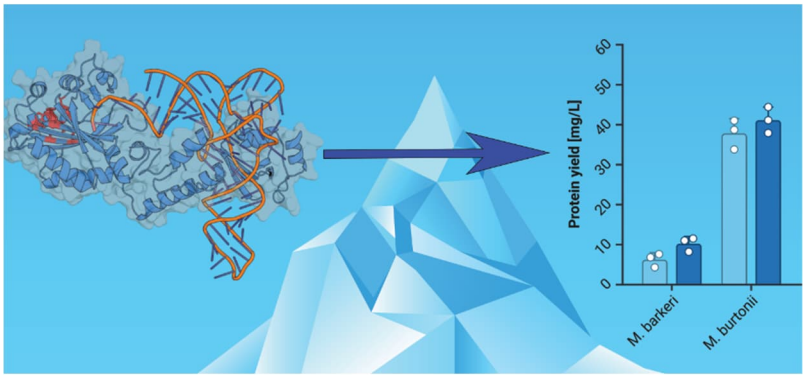
INTRODUCTION:

Aminoacyl-tRNA synthetases (aaRSs) are vital enzymes that ensure precision in translating the genetic code by attaching specific amino acids to their corresponding tRNAs. The natural genetic code limits the range of canonical amino acids permitted for ribosomal translation. Expanding this repertoire beyond the standard 20 necessitates altering the substrate specificity of aaRSs, as they play a fundamental role in interpreting the genetic code.

PROJECT:

Over 200 non-canonical amino acids (ncAAs) have been incorporated into proteins using diverse genetic code expansion methods, including selective pressure incorporation, stop codon suppression, fragment condensation, protein semisynthesis, and peptidomimetics. These ncAAs, with non-proteinogenic functional groups, offer tools to manipulate and explore various aspects of protein biology, including structure, dynamics, function, interactions, catalysis, folding, synthesis, trafficking, degradation, and aggregation.

The proposed research will establish a cutting-edge learning environment for students to delve into directed enzyme evolution. This will involve testing and enhancing existing enzymes, as well as screening orthogonal pairs of aminoacyl-tRNA synthetase (aaRS) and tRNA from available sources for beginners. Advanced students will design enzyme and tRNA libraries to further expand their understanding and skill set in this field. technologies.



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3. H Sun, Jia, H., O. Kendall et al. & N. Budisa (2022) Halogenation of tyrosine perturbs large-scale protein self-organization. *Nature Communications*, 13, 4843 (https://doi.org/10.1038/s41467-022-32535-2)

Project #6:
Photoaminocatalysis Design and Development

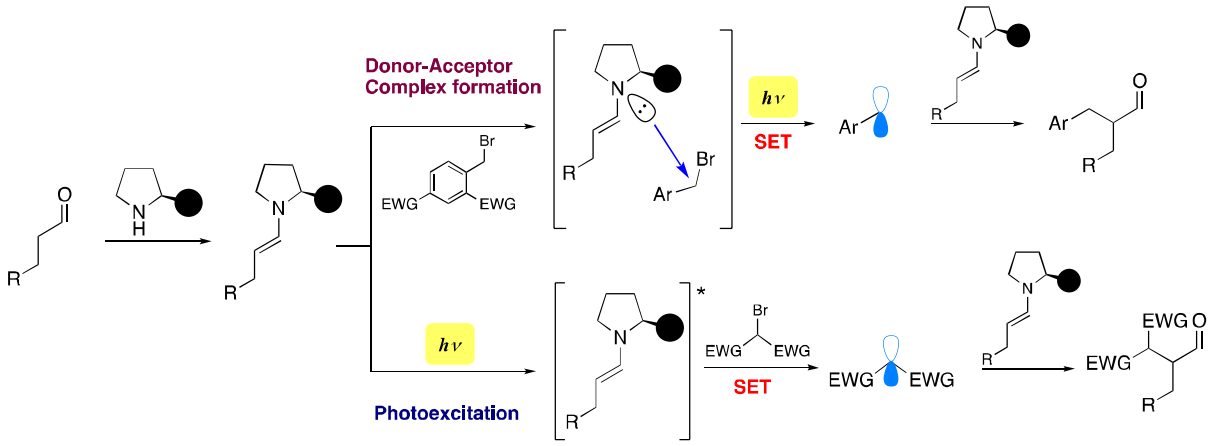
Dr. Rebecca Davis (Rebecca.Davis@umanitoba.ca)

INTRODUCTION:

Photo-organocatalysis is set to be the next major advancement in the field of asymmetric synthesis and provide access to previously unachievable transformations. Recently it has been demonstrated that organocatalytic enamine intermediates can interact with visible light to directly activate substrates via single electron transfer (SET). The photocatalytic activity of these enamines holds great promise for the development of new asymmetric, regioselective reactions.

PROJECT:

The proposed work aims to determine the influence of the catalyst scaffold on promoting SET processes and identify what features should be considered when designing a photocatalyst or a photocatalytic reaction. Employing a combination of spectroscopic studies and theoretical calculations on the reactive enamine intermediates, formed from a range of chiral secondary amines, we will be able to establish which features of the catalysts are responsible for the absorption properties of the enamines. The results provided by these studies will serve to guide our reaction and catalyst design efforts and aid in the application of this methodology in new stereoselective γ- and ε-addition reactions. The student involved in this project will begin by using DFT methods to understand the interactions of the catalysts and substrates they will later move into the lab to study these interactions using state of the art spectroscopic methods including in situ IR and NMR flash photolysis.



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1) Silvi, M., and Melchiorre, P. Enhancing the potential of enantioselective organocatalysis with light *Nature,* 2018*, 554*, 41-49.

2) Lima, C. G. S., Lima, T. de M., Duarte, M., Jurberg, I. D., Paixao, M. W. Enabled by Light-Irradiation of EDA Complexes: Theoretical Background and Synthetic Applications, *ACS Catal.* 2016, Volume 6, 1389-1407.

Project #7:
Drug Discovery with Machine Learning

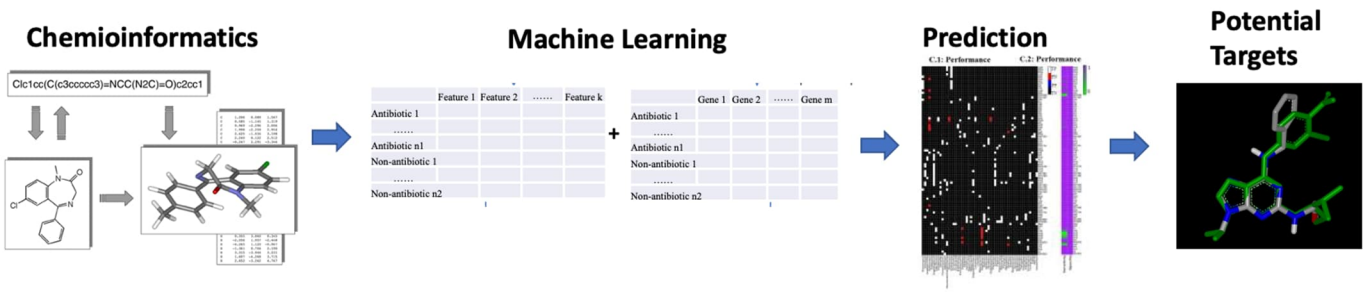
Dr. Rebecca Davis (Rebecca.Davis@umanitoba.ca)

INTRODUCTION:

The emergence of multidrug-resistant bacterial infections is a major modern health threat. Infections caused by Gram-negative bacteria are more worrisome as their cell envelopes are less permeable to antibiotics. Consequently, the development of novel antibiotic discovery strategies tailored to Gram-negative bacteria is a pressing need. As part of a multidisciplinary team, the Davis group is working to develop a deep learning tool to predict antibiotic activity.

PROJECT:

The proposed work aims to both work on the generation of small molecule libraries for screening and identification of potential antibiotics as well as to determine what features of molecules are necessary to determine antibiotic activity (helping to answer the question: How do we teach computers chemistry?). The student involved in this project will learn a variety of chemioinformatic tools to analyze small molecule libraries. This includes everything from standard ADMET property generation to the many features implemented in RDKit. We will also use 3D structure -specific features to describe antibiotics and non-antibiotics and link the compounds' 3D structures with chemogenomic profiles by using AI-based deep learning model.



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Project #8:
Polarized infrared spectrochemical imaging and Two-Dimensional Correlation spectral analysis of polymer biodegradation

Dr. Kathleen M. Gough (kathleen.gough@umanitoba.ca, (204) 474-6262)

INTRODUCTION:

Pollution caused by fossil fuel-based plastics is a major environmental concern.[1] Polylactic acid (PLA), a bio-based polymer, is often viewed as an environmentally friendly, practical alternative to petrochemical plastics,[2] as it possesses many of the desirable physical and mechanical characteristics, is bio-synthesized, and can be degraded by hydrolysis and microbial action. Unfortunately, complete biodegradation of PLA is still very challenging. Specific controlled conditions of temperature, humidity, pH and bio-organisms are required. Even then, the process is slow and incomplete as the crystalline phase is less susceptible to chemical and biochemical attack. Infrared vibrational spectroscopy,[2,3] offers a direct window into the state of PLA films, letting us evaluate of the efficacy of modified and novel treatments, *in vitro* and in composting systems,[4] with the goal of enhancing the biodegradation rate of PLA.

PROJECT:

Commercial PLA-containing products have variable characteristics and composition. For this controlled study, you will prepare pure spin-cast PLA films. Infrared (IR) vibrational spectroscopy is widely used on polymer films such as PLA.[2] Since the raw spin-cast PLA is entirely amorphous, you will experiment with annealing at higher temperatures to create different degrees of crystallinity that can be directly assessed with a combination of advanced IR techniques, including imaging, polarized IR, and 2D-COS analysis.[3] The latter analysis is applied to set spectra from the same sample acquired under external sample perturbations, such annealing at different temperatures for different periods of time or cooling conditions. With the 2D-COS software, you will plot the correlated spectral changes as a function of treatment and time sequence. You will be able to monitor the effect pre- and post-treatments[4] by re-examining the treated films using the same IR techniques. You will be part of an interactive team, working directly with students in my group, as well as interacting with students and professors who are involved in the campus-wide Prairie iGEM (International Genetically Engineered Machine) team. This project will give you a chance to work on problems of global environmental significance, and to gain experience in experimental techniques that are widely used in research and industry.

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2. Yan, J. et al. 2023. Application of infrared spectroscopy in the multiscale structure characterization of poly (L-lactic acid), *Polymer* 278 (2023) 125985.z
3. Park Y, Noda I and Jung YM (2015) Two-dimensional correlation spectroscopy in polymer study. *Front. Chem*. 3:14.
4. Mohanan N; Wong N C-H; Budisa N; Levin DB (2023) Polymer-degrading enzymes of *Pseudomonas chloroaphis* PA23 display broad substrate preferences. *Int J Mol Sci* 24:4501.

Project #9:
Assessment of possible repair mechanisms of ancient parchment
Infrared vibrational spectroscopy

Dr. Kathleen M. Gough (kathleen.gough@umanitoba.ca, (204) 474-6262)

INTRODUCTION:

Parchment, a complex biological material made from processed animal skins, was widely used as a writing medium across Europe, the Mediterranean, and the Horn of Africa from the 2nd century BC. Historically significant documents, e.g: the Magna Carta[1], are kept under strict environmental control to preserve these precious, unique, cultural and historical artifacts from our past. Despite its longevity, parchment is susceptible to collagen-specific degradation mechanisms. Our 5-year NSERC Discovery Horizons project "Archival Parchments Rejuvenation: Re-engineering native collagen crosslinks for the test of time", led by Prof. Laurent Bozec (UToronto) was funded in spring 2023. Our proposal focuses on re-engineering natural glycation crosslinks in collagen in parchment using methods translated from Tissue Engineering in the Bozec lab. As a co-investigator, Kathy Gough is using her expertise in infrared spectroscopy of collagenous materials to evaluate the damaged parchments and the effectiveness of the novel chemical treatments that are being developed in the Bozec lab, with the long-term goal of designing a process for repair of model parchments.

PROJECT:

Parchment samples to be studied include new parchment materials (full hide calf skin; Pergamena, USA) and the collection of historical parchments originating from the EU-funded Improved Damage Assessment of Parchment (IDAP) project. The unique triple helical structure of collagen at the molecular level translates into an unusual and very characteristic IR spectrum that conformation- and orientation-dependent in normal tissues and measurable at the micro-[2] to nano-scale[3]. You will prepare collagen extracts from parchments supplied by the Bozec lab and examine them with high spatial resolution (1.5 micron) FTIR spectrochemical imaging using our IR microscope with focal plane array detector. You will do experiments using near-field nano-IR spectroscopy at the nanoscale, conducted through remote access to the IR beamlines at the Advanced Light Source, Berkeley, USA. You will participate in a collaborative, multi-team, cross-disciplinary study that is significant in that it addresses the urgent need of museum curators and conservators for long-term solutions to preserve parchment as a cultural heritage. You will learn the technical aspects of polarized Infrared spectroscopy and imaging, a technique that it being used in field from industry to health care.

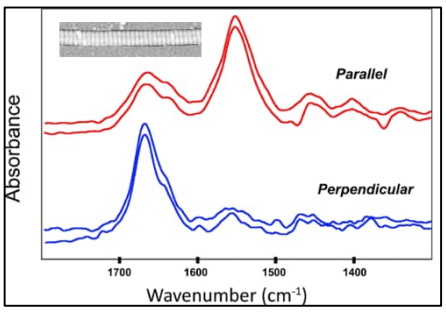

Fig. 1: Spectra of collagen fibrils under polarized IR light.[2]

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2. G Bakir, BE Girouard, R Wiens, S Mastel, E Dillon, M Kansiz, K Gough," Orientation Matters: Polarization Dependent IR Spectroscopy of Collagen from Intact Tendon Down to the Single Fibril Level" *Molecules* 25:4295 (2020)
3. R Wiens, CR Findlay, SG Baldwin, L Keplak, J Lee, S Veres, KM Gough, *Farad Discuss*, 187:555-573 (2016)

Project #10:
Bone chemical composition analysis for personalized bio-printed orthopedics

Dr. Kathleen M. Gough (kathleen.gough@umanitoba.ca, (204) 474-6262)
Dr. Christian Kuss (christian.kuss@umanitoba.ca, (204) 480-1823)

INTRODUCTION:

Hip fractures represent a significant health concern among the elderly population and often lead to substantial health complications[1]. Recognizing the pressing need to enhance the treatment outcomes for individuals with hip fractures, the University of Manitoba recently funded an Ignite project focusing on the bioprinting of orthopedic devices[2]. This ground-breaking endeavor aims to revolutionize orthopedic care by developing personalized solutions tailored to individual patient needs. Central to the success of this initiative is a comprehensive understanding of bone composition and its relationship to mechanical properties. This student project integrates with this new research program, by determining bone composition using infrared vibrational spectroscopy, ICP-OES spectroscopy, and electron microscopy.

PROJECT:

Dehydrated bone predominantly consists of a mineral matrix of hydroxyapatite and an organic matrix[3]. The major components of the mineral matrix are calcium and phosphate but may also include magnesium, sodium, potassium, fluoride, zinc, and other minor components. This component imparts hardness to the bone. The organic matrix is dominated by collagen, which supports both flexibility and strength. ICP-OES spectroscopy will allow the determination of the mineral composition of the bone. The distribution of these elements across the bone sample will be determined by electron microscopy imaging. Infrared vibrational spectroscopy will be used to understand the organic composition of the samples[4]. You will share your findings with the rest of the Ignite team, providing essential insights into the bone composition. These insights will then be correlated with mechanical studies conducted on the same samples by other Ignite team members, forming a cohesive understanding of the bone structure and function. The ability to extrapolate the chemical composition of a patient's bone sample to its mechanical properties is a crucial cornerstone for tuning the composition of replacement materials used in the targeted bio-printing process. As such, this project offers you the opportunity to participate at the very origin of a potentially life-changing new orthopedic technology while learning crucial and transferable analytical skills.

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Project #11:
Photocatalysis Using Designer Sustainable Chromophores

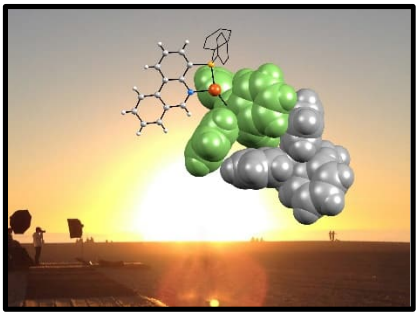
Herbert (david.herbert@umanitoba.ca, (204)474-7535)
Group Website: http://home.cc.umanitoba.ca/~dherbert/

INTRODUCTION:

As the world's population grows, so too does the global demand for materials and energy. The ability to harvest solar energy (solar cells) and manipulate light output (display technologies and low-cost/energy usage lighting) using *abundant* materials will be key to providing a high global quality of life to as many people as possible, while limiting the impact of making and using these materials on our climate and environment. A very promising additional application is to use molecules to *catalyze* reactions leveraging sunlight in place of thermal energy ("photocatalysis").

PROJECT:

As part of our group's broader efforts to target new dyes to harvest solar energy based on abundant elements such as iron (Fe), and new emissive materials based on copper (Cu) and zinc (Zn), we are designing ligand motifs for transition metals and constructing their transition metal coordination complexes, where we modify the molecular structure of ligands through chemical synthesis in order to tune the photophysical and electrochemical properties of complexes. In doing so, we target molecules that can absorb a broad range of the electromagnetic spectrum across the visible and, ideally, into the near-IR, and allow for tuneable emission from complexes of abundant metals.



This project takes our work to the next level by evaluating some of our molecules in photocatalytic reactions. A 4710 student will work directly alongside Dr. Herbert and a graduate student mentor to construct chromophores and using our photoreactor, examine their utility in photocatalysis.

REFERENCES:

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C.B. Larsen, J.D. Braun, I.B. Lozada, K. Kunnus, E. Biasin, C. Kolodziej, C. Burda, A. Cordones, K. Gaffney, D.E. Herbert *J. Am. Chem. Soc.* 2021, *143*, 20645

R.J. Ortiz, J.D. Braun, J.A.G. Williams, D.E. Herbert *Inorg. Chem.* 2021, *60*, 16881

Project #12:
Scaffold Hopping by Photochemical Carbon Deletion from Benzannulated Azaarenes

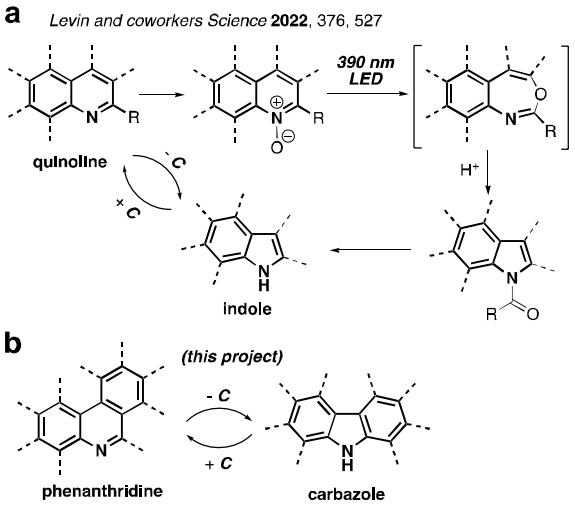
Dr. David Herbert (david.herbert@umanitoba.ca, (204)474-7535)
Group Website: http://home.cc.umanitoba.ca/~dherbert/

INTRODUCTION:

Chemists often identify molecular structures that show promise for a specific application, for example, as chemotherapeutics, molecular electronics, or solar materials. The preparation of each new candidate molecule in a series can often require a completely new synthetic approach if the core of the molecule needs to be altered. Synthetic methodologies that can easily and directly interconvert between molecular cores are tantalizingly attractive ways to streamline molecular discovery.

PROJECT:

Very recently, chemists at the University of Chicago reported[1] an exciting new approach to 'hop' directly between chemically distinct heteroaromatic scaffolds, namely quinoline *N*-oxides and *N*-acylindoles (a). We have developed synthetic routes to functionalized phenanthridines, also known as benzo[c]quinolines,[2] and demonstrated their use in diverse applications including as emissive materials.[3] This project will involve applying this scaffold hopping protocol to convert phenanthridine *N*-oxides to carbazoles to investigate the extension of this exciting work to *benzannulated* azaarenes (b).



This project requires an enthusiastic and engaged student interested in sustainable chemistry and learning about synthetic organic chemistry, in particular the use of photochemistry. A 4710 student will work directly alongside Dr. Herbert and a graduate student mentor to develop an optimized protocol for ring-contraction starting with 6-methyl phenanthridine *N*-oxide. The starting materials will be characterized using multinuclear NMR and UV-Vis absorption spectroscopy. A photochemical protocol using an LED photoreactor will be developed, and products isolated and analyzed chemically. Once an optimized procedure is established, the 4710 project will then look to establish a substrate scope for this transformation using a library of phenanthridine *N*-oxides prepared using our pre-existing library of available substituted phenanthridines.

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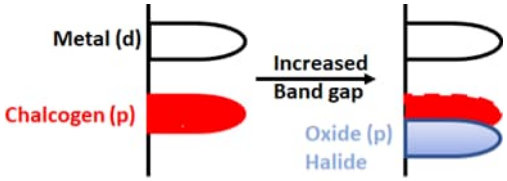
Project #13:
Discovery of new heteroanionic compounds to enhance optical properties

Dr. Abishek Iyer (abishek.iyer@umanitoba.ca, https://www.iyerlab.ca/
(204) 474 7346)

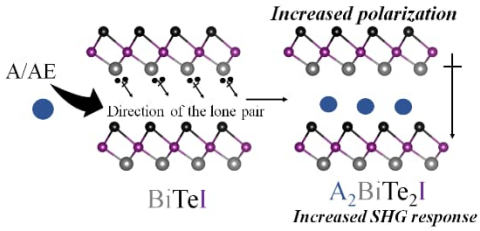
INTRODUCTION:

The lack of new materials in the IR region is limiting the development lasers and light emitting diodes (LED), with the expected market revenue of IR devices to reach $1550 millions by 2027. Chalcogenides (*Q*) and pnictides (*Pn*) are transparent in the IR region but have low bandgaps (< 2 eV), leading to low laser-induced damage threshold (LIDT) at high laser powers. One key aspect to tuning the bandgap is through the introduction of multiple anions or heteroanions which can result in flattening the band dispersion in the electronic band structure there by increasing lowering the valence band and increasing the overall bandgap. Chalcohalides (compounds containing chalcogens and halides) have been studied as promising materials for LED ($Rb_6Re_6S_8I_8$), solar cells (BiSeI) and nonlinear optics ($Ba_4Ge_3Se_9Br_2$).



PROJECT:

The project will focus on the discovery of new chalcohalides by developing rational synthetic designs. The synthesis of chalcohalides will be approached using both solid-state and hydrothermal methods to study the effect of temperature on the crystal structure. The charge mismatch between the halides (X^{-1}) and the chalcogen (Q^{2-}) hinders direct site-substitution. Instead, we will combine alkali (*A*)/alkaline earth-metals (*AE*), streochemically active lone pair (SALP) containing cation (Bi or Sb) and heteroanions (chalcogens and halides) to tailor new crystal structures from known building blocks. The hard anion would preferentially bond to *A*/*AE* and distort its polyhedra. The SALP on the second cation will also play a role in distorting the polyhedra. We will explore a series the insertion of AEX slabs (fluorite structure-type) in-between Bi*Q*I and In_5Q_5X, respectively. The materials will be characterized using X-ray diffraction (powder: phase identification; single: crystal structure determination), diffuse reflectance (band gap determination) and differential scanning calorimetry (DSC: melting behavior). Once the single crystal structure is obtained, we will be able to apply these materials to specific applications such as nonlinear optics if the structure is noncentrosymmetric (lacking a center of inversion). The project will offer an opportunity to integrate synthetic inorganic chemistry with materials chemistry.



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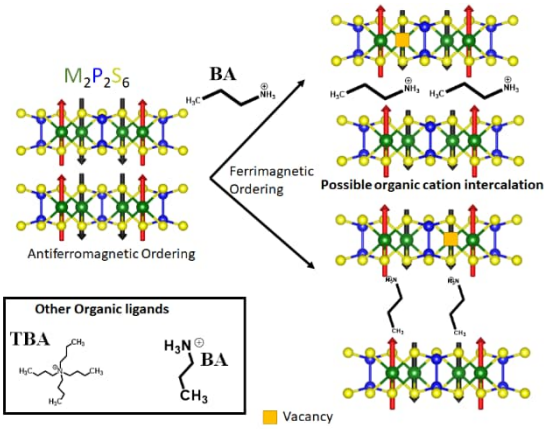
Project #14:
Tuning magnetism among 2D magnetic materials through organic cation intercalation

Dr. Abishek Iyer (abishek.iyer@umanitoba.ca, https://www.iyerlab.ca/
(204) 474 7346)

INTRODUCTION:

Spintronics is a newly developing field that uses the spin of the electron and the associated magnetic moment for developing next-generation efficient electronics like quantum computing. Efficient computing requires electronics made up of materials where electron spins can be used for data storage and exchange at room temperature. However, the development of this field is restricted by the availability of room-temperature ferromagnetic 2D materials. Metal chalcophosphate systems like $M_2P_2Q_6$ (M = transition metals, Q = S, Se), $MM'P_2Q_6$ (M = alkali, Cu and Ag and M'= 3+ transition and rare-earth metals) and $MM'P_2Q_7$ (M = alkali, Cu and Ag and M'= 3+ transition and rare-earth metals) are a family of layered materials which order anti-ferromagnetically. This family of compounds have a large structural diversity wherein they can accept multiple cations as long as they add up to 4+. Doping of these materials with inorganic cations has been extensively studied however, to limited success in tuning the magnetic ordering temperatures.

PROJECT:



The project will focus on developing design principles for tuning the magnetic properties by intercalating organic cations in these chalcophosphate systems. The bulk material will be synthesized using P_2Q_5 flux as reported in literature.2 The organic cation intercalation will be achieved via hydrothermal synthesis and/or electrochemical synthesis. We will start with the effect of intercalation due to length of organic cation like methyl (MA), formamidium (FA) and tert-butyl ammonium (TBA) cations and study the change in structure using X-ray diffraction and electron diffraction (ED). Powder x-ray refinements will provide structural information where the (00*l*) reflections will be compared with the pristine sample for any shifts to confirm the intercalation has worked. Once the organic cation intercalation is confirmed then their bulk magnetic properties will be measured to confirm their magnetic ordering. The project will offer an alternative way of tuning magnetic ordering in promising 2D materials.

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Project #15:
Ion-Exchange in metal-sulfides for water remediation

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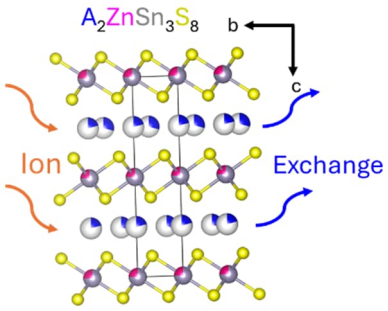
(204) 474 7346)

INTRODUCTION:

Local water bodies are commonly contaminated with complex mixture of metal pollutants originating from diverse industrial activities including mining operations, metal plating facilities, and tanneries. These pollutants make the water very acidic and fill them heavy metal ions such as Cu^{2+}, Fe^{3+}, Mn^{2+}, Zn^{2+}, Cd^{2+} and Pb^{2+}. These which tend to accumulate in living organisms, causing various diseases and disorders. The issue is worse in closed and abandoned mines where water stays stagnant. Efficiency of commonly used sorbents such as clay/earth-based minerals; zeolites; and fly ash are influenced by pH or initial contaminant concentrations. Certain two-dimensional (2D) metal-sulfides have shown promising ion-exchange capabilities and stability across a broad pH spectrum. This is primarily due to the concept of hard-soft acid-base principles.

PROJECT:



S^{2-} being a soft Lewis-acid exhibits a strong interaction with other softer Lewis bases like Hg^{+}, Pb^{2+} and Cd^{2+}. The idea of the project will be to synthesize novel layered metal-sulfides using inexpensive starting materials (carbonates/acetates) synthesized using hydrothermal methods. We will look to synthesize new compounds like $A_2ZnSn_2S_6$ and $A_2ZnSn_3S_8$ (A = Na and K) using a Parr bomb hydrothermally. The formation of the compounds will be confirmed using powder X-ray diffraction (pXRD) and inductively coupled plasma optical emission spectroscopy (ICP-OES) for elemental analysis. After structural conformation the stability of the materials will be performed at different acidic pH. After which ion exchange will be performed at different pH and different times. The ion-exchange will be characterized using pXRD where shifts in the (00l) Braggs reflections, color changes in the solids and ICP-OES will be performed. Different metal mixtures will be studied for selectivity studies, the effect of ion-exchange on the structure of the material used and the reusability of the ion-exchanger. The project will offer the student an opportunity to integrate inorganic chemistry with physical and analytical chemistry.

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Project #16:
Investigating the folding of paratox

Dr. Khajehpour (Mazdak.Khajehpour@UManitoba.ca, (204) 2721546)

INTRODUCTION:

Paratox is a small protein that acts as an inhibitor of new DNA acquisition by streptococci bacteria. In this project we plan to study the folding thermodynamic and kinetic properties of paradox in order to understand the folding mechanism of this protein.

PROJECT DESCRIPTION:

In this project the student will learn how to over-express and purify paratox. They would then determine the thermodynamic parameters of the protein folding process using differential scanning calorimetry (DSC) and chemical denaturation methods. From these measurements the ΔH, ΔS, ΔG and ΔC_p of the protein will be determined. The folding mechanism of paratox will be studied through fast denaturation methods using stopped flow kinetics. These measurements will determine the number of intermediate steps involved in the protein folding process and the folding and unfolding rate constants. The effects of salts, osmolytes and pH on the kinetics and thermodynamics of the paratox folding process will also be determined. In addition to DSC and stopped flow the student in this project will also learn how to use and interpret steady-state and time-resolved fluorescence spectroscopy, as well as circular dichroism spectroscopy.

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Project #17:
Selection of ribosomal RNA sites by H/ACA small nucleolar Ribonucleoproteins for ribosome synthesis

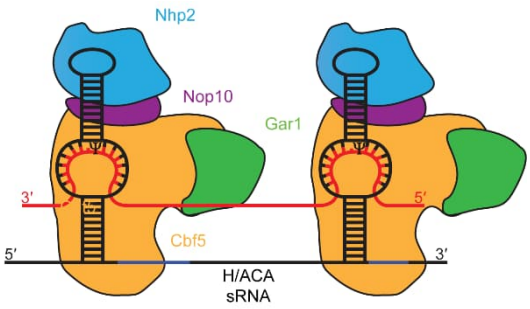
Dr. Ute Kothe (Ute.Kothe@UManitoba.ca, (431) 371 0878)

INTRODUCTION:

Ribosome assembly is a multistep process that generates the cell's protein synthesis machinery called ribosome which is composed of both large ribosomal RNAs (rRNA) and many proteins. Furthermore, hundreds of additional proteins and small nucleolar RNAs (snoRNAs) assist with ribosome biogenesis by transiently interacting with ribosome precursors. The Kothe group aims to understand the molecular mechanisms how these proteins and snoRNAs facilitate ribosome assembly with the long-term goal of identifying strategies to inhibit ribosome formation in rapidly growing cancer cells.

PROJECT:

H/ACA snoRNPs are versatile molecular machines that are composed of an H/ACA snoRNA and a core set of four H/ACA proteins. The snoRNA facilitates base-pairing with ribosomal RNA whereas the H/ACA protein called Cbf5 in yeast (dyskerin in humans) is responsible for site-specifically modifying a uridine in ribosomal RNA to pseudouridine. Moreover, H/ACA snoRNPs can unfold structures in ribosomal RNA likely prevent mistakes during ribosome synthesis.



The objective of this project is to investigate how H/ACA small nucleolar Ribonucleoproteins (snoRNPs) select sites in ribosomal RNA for binding and potential pseudouridylation. In addition to base-pairing with the target site for pseudouridine formation, the Kothe lab has recently shown that H/ACA snoRNPs can also bind to other regions of ribosomal RNA. You will investigate how these "near-cognate" sites compete with the cognate target sites in binding to H/ACA snoRNPs. To dissect the function and the mechanism of H/ACA snoRNP interactions with ribosomal RNA, you will purify both proteins and RNAs. The binding of RNA to H/ACA proteins and the H/ACA snoRNP complex will be assessed by different methods such as affinity chromatography, (q)RT-PCR and fluorescence.

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Czekay, D. P., Kothe, U. (2021) H/ACA Small Ribonucleoproteins: Structural and Functional Comparison Between Archaea and Eukaryotes. *Frontiers in Microbiology, Vol. 12, Article 654370*

Kelly, E., Czekay, D.E., and Kothe, U. (2019) Base pairing interactions between substrate RNA and H/ACA guide RNA modulate the kinetics of pseudouridylation, but not the affinity of substrate binding by H/ACA small nucleolar Ribonucleoproteins *RNA* 25 (10), pp. 1393 – 1404, doi: 10.1261/rna.071043.119

Project #18:
Biologically Active Glasses for Soft-Tissue Wound Healing

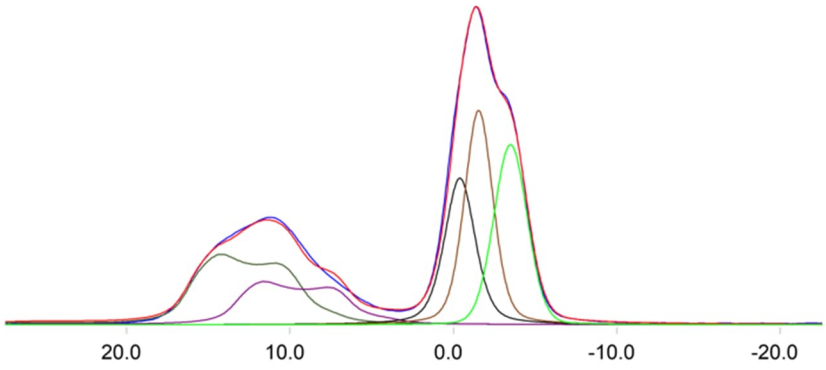
Dr. Scott Kroeker (Scott.Kroeker@UManitoba.ca, (204) 474 9335)

INTRODUCTION:

Glasses are becoming widely used for bone reconstruction and soft-tissue wound healing. Biologically active glasses dissolve in bodily fluids and deposit as bone minerals, or deliver therapeutic ions to wound sites. Which of these functions occurs depends on the dissolution properties of the glass, which depend in turn on the glass composition and structure. This project uses nuclear magnetic resonance (NMR) spectroscopy to study the structure of novel glasses with potential biomedical applications to determine the key structural parameters governing the dissolution of bioactive glasses.

PROJECT:

Borophosphate glasses will be prepared by high-temperature synthesis, followed by analysis using ^{11}B, ^{23}Na, ^{31}P, ^{29}Si and ^{27}Al NMR spectroscopy. Spectral interpretation yields the identities and amounts of different glass components, which are used to define the connectivity patterns that make up the glass network. The chemical durability of these glasses will be evaluated in dissolution trials, and elemental release measured by ICP-OES as a function of time. The transformation of the materials during dissolution will be characterized by NMR spectroscopy and complementary methods such as scanning-electron microscopy. By correlating structural changes with properties such as dissolution behaviour and crystallization, a deeper understanding of how properties depend on glass composition can be established to aid the design of bioactive glasses which require the smooth release of therapeutic ions near the injury site for soft-tissue wound healing. Projects can be tailored to student interests and strengths to emphasize synthetic, analytical or physical aspects of these projects.



^{11}B magic-angle spinning NMR of a borophosphate glass with two types of BO_3 and three types of BO_4 units.

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Project #19:
Surface Corrosion of Nuclear Waste Glasses

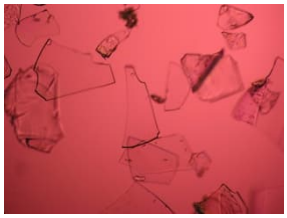
Dr. Scott Kroeker (Scott.Kroeker@UManitoba.ca, (204) 474 9335)

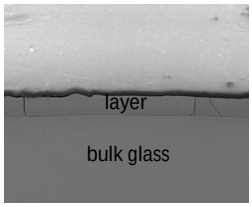
INTRODUCTION:

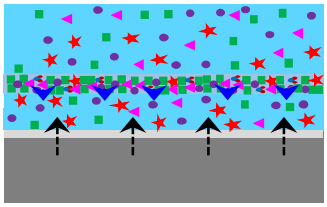
The safe disposal of nuclear waste requires chemically durable materials which retain radioactive species for hundreds of thousands of years in geological environments. Choosing a suitably durable glass composition is fundamental to success, but it has recently been found that interaction with aqueous solution transforms the surface of the glass into a protective layer which adds a further barrier to radionuclide release. Unfortunately, the layer formation and properties are poorly understood and very difficult to study. We have found a way to grow surface layers on (inactive) glasses which mimic nuclear materials so we can study their structural characteristics with solid-state nuclear magnetic resonance (NMR) spectroscopy.

PROJECT:

Borosilicate glasses will be prepared by high-temperature synthesis and exposed to aqueous solutions to effect surface alteration. Analysis of the altered materials by ^{11}B, ^{23}Na, ^{29}Si and ^{27}Al NMR spectroscopy will provide information about the identities and amounts of different glass components, which can be compared with those found in the original unaltered glasses. Surface-sensitive NMR methods will be used to dinstiguish the structure of the layer from the underlying bulk glass structure. The layer morphology and elemental composition will be characterized scanning-electron microscopy to better understand the formation mechanism. Elemental release will be measured by ICP-OES as a function of time to better understand the protective function of the layer. Learning more about the formation, structure and properties of glass corrosion will aid in predicting the long-term behaviour of materials for radioactive immobilization, and in designing better glasses to maximize environmental isolation. This project can be tailored to student interests and strengths to emphasize synthetic, analytical or physical aspects.







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Project #20:
Catching Batteries in the Act:
Operando Characterization of Battery Materials

Dr. Christian Kuss (christian.kuss@umanitoba.ca, (204) 480-1823)

INTRODUCTION:

When batteries charge or discharge, a large number of dynamic processes occur. The resulting transient properties of the materials that make up the battery control the battery performance. In contrast, outside the operating battery, the materials are static and stable. Therefore, the characterization of these materials outside the battery often reveals an incomplete or inaccurate picture of their performance contributions during operation. Enter operando characterization – the application of analytical tools to an operating device[1]. In this project, you will explore the operando characterization of a battery material with brand-new, state-of-the-art material characterization tools.

PROJECT:

Binders are crucial materials in batteries that adhere the charge-storing active materials to the electrode. Battery failures are often associated with binding problems. In 2019, the Kuss group developed a new conductive binder material for use in next-generation batteries that is more adhesive, can be processed in water (rather than toxic solvents), and is electronically conductive, improving the fast-charging performance of batteries[1]. To support the characterization of these binders and to understand their performance and limitations, recent funding from the Canada Foundation for Innovation has brought new operando characterization equipment to the Kuss group. You will choose whether to explore these new battery materials using operando infrared, Raman, or UV/Vis spectroscopy. The results will yield information on the dynamic behavior of these binders and their chemical environment, as well as their chemical stability and performance. The resulting data will inform the selection of the most appropriate next-generation battery technologies for the application of the Kuss group's novel conductive binders and underpin the development of new binders.

Figure 1 Recently installed FTIR spectrometer and operando electrochemical cell within Argon glovebox, waiting to be used.

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Project #21-A:
Single-Entity Electrochemistry

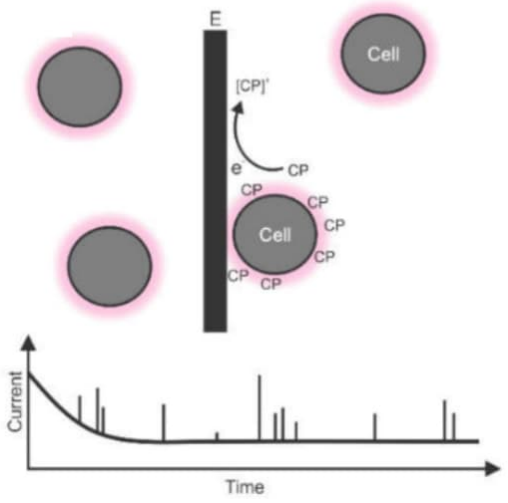
Dr. Sabine Kuss (sabine.kuss@UManitoba.ca, (204) 272 1693)

INTRODUCTION:

Impact electrochemistry is a powerful technique for the detection of single entities.[1,2] In the literature, its main application is related to the detection and characterization of nanoparticles in solution.[3] This project explores the application of impact electrochemistry to biological organisms to detect pathogens in aqueous solutions, but also to quantitatively assess cellular features, such as molecule efflux across cell membranes. If successful, this study will demonstrate the immense potential of single-entity electrochemistry as a revolutionary tool in biosensing.

PROJECT:

Impact electrochemistry is based on the faradaic charge transfer, following the collision of redox-active entities with an electrode. Governed by diffusional Brownian motion, single particles collide with an electrode, which is held at an oxidizing or reducing potential of a redox species. Thereby, entity impacts at the electrode result in short current bursts ("spikes"). To date, no redox active cell metabolite has been reported for the application to impact electrochemistry, but methodologies involving nanoparticle-labeled bacteria and their detection through an electrochemical "off"-signal have been proposed.[4,5] In this project, the cell metabolite glutathione, the efflux of antibiotics from bacteria, and the efflux of chemotherapeutics from living cancer cells will be studied (scheme 1). All of these three cellular events are intrinsically connected to drug resistance mechanisms of cells, as drugs are commonly expelled from the cell interior through active pumps, either in conjugation with glutathione or on their own. If successful, this methodology will not only detect pathogens in aqueous solutions at high throughput rates, but will also enable the quantification of drug resistance phenotypes in bacteria and cancer.



Scheme 1: Living cells collide with an electrode during impact electrochemistry. The efflux of the chemotherapeutic carboplatin (CP) results in current spikes.

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Project #21-B:
Electrochemical Detection of Mycotoxins in Canadian Grain

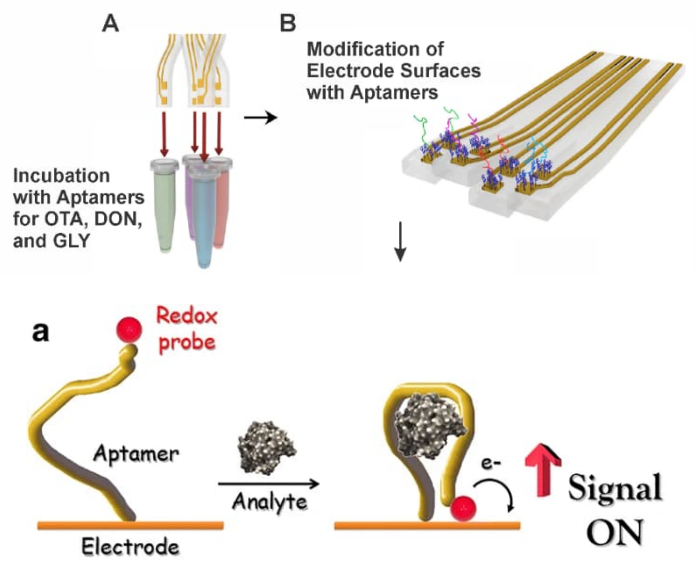
Dr. Sabine Kuss (sabine.kuss@UManitoba.ca, (204) 272 1693)

INTRODUCTION:

Mycotoxins, such as ochratoxin A (OTA) and deoxynivalenol (DON) are prevalent contaminants in Canadian grain and cause devastating losses for grain producers across Canada.[1] Grain that is intended for human consumption, but also animal feed is susceptible to contamination with mycotoxins. Current multi-analyte tests require costly scientific instrumentation, laboratory equipment, and expertise. Electrochemistry can offer portable, inexpensive, and fast alternative methods. The aim of this project is to detect at least two grain contaminants simultaneously using disposable screen-printed electrodes that can be implemented into a micro-fluidic device for the detection of mycotoxins in Canadian grain.

PROJECT:

As shown in scheme 1, this project involves structure-switching electrochemical aptamer sensors. Individual electrode arrays are incubated with aptamers specific for relevant grain contaminants. A DNA or RNA aptamer structure is bound to a gold electrode surface and tagged with the redox probe methylene blue. The aptamer-modified electrodes will be exposed to solutions of OTA and DON. Upon binding of target analytes, folding of the aptamer structure brings the redox tag in close proximity to the gold, enabling faster electron transfer and an increase in electrochemical current during voltammetric measurements. Upon successful detection of OTA and DON in a buffer, real grain samples will be analyzed in collaboration with the Canadian Grain Commission. Mycotoxins will be extracted from grain matrices by washing and the design of a microfluidic flow-through chamber for high throughput analysis will be explored.



Scheme 1: (A) Mycotoxin-specific aptamers will bind to gold coated electrochemical arrays (B).[2] A redox probe is attached to the aptamer (a), and upon binding of OTA or DON, folding of the aptamer structure brings the redox tag near the gold, enabling faster electron transfer.[3]

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Project #22:
Chemistry Outreach in Manitoba: Life Beyond the Perimeter

Dr. Joey Lussier (Joey.Lussier@UManitoba.ca, (204) 474-7652)

INTRODUCTION:

Chemical literacy is becoming progressively more important as environmental consequences of resource management and sustainable energy development have increasing impacts on society. Unfortunately, students from rural and Indigenous communities often are disadvantaged because of a lack of laboratory infrastructure and may not be taught by experts (e.g. trained chemists). Furthermore, it becomes more difficult to effectively educate students in the hands-on techniques required in chemistry when resources and services found in large cities are not easily accessible. Consequently, students entering university from communities outside of larger cities/centers often struggle with their first years in chemistry. The goal of this chemical education project is to identify and address some of these issues both in the communities, and in the university curriculum.

PROJECT:

In this project a chemistry outreach program will be developed with a focus on rural and Indigenous communities in Manitoba. The goal of this project is twofold; a) to spark an interest in chemistry and engage Indigenous students and b) integrate Indigenous Knowledge into university chemistry.

Step one involves building partnerships with rural and Indigenous communities and working together with champions in the community (Elders, teachers, or other community members). Concerns of access to chemistry resources will be identified using qualitative and quantitative methods. This project will use an approach of two-eyed seeing[1] to blend Indigenous Ways of Knowing with western science to decolonize the current approach to scientific education. The project may include the development of new experiments, alternative lessons or lectures, and new tutorial formats. Consequently, this will spark an interest in chemistry in more students from diverse backgrounds. The knowledge gained will also flow into introductory university chemistry courses. The material will be a resource to the department of chemistry and will be included in new course development. The project student will gain many skills in the scholarship of teaching and learning, with a strong emphasis on chemical education beyond the traditional university approach.

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Project #23: Characterization of RNA-Protein Complexes that Regulate Translational Control

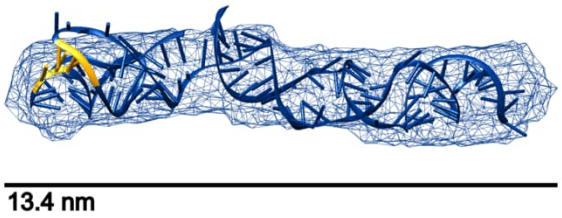
Dr. Sean McKenna (Sean.McKenna@Umanitoba.ca)

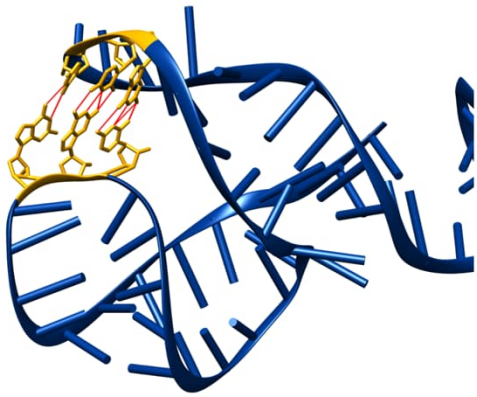
INTRODUCTION:

Brain Cytoplasmic RNA 1 (BC200) is a 200 nucleotide long non-coding RNA that is hypothesized to regulate protein translation and play a key role in regulating carcinogenesis. We have begun to define the BC200-containing protein complexes that mediate BC200 function through immunoprecipitations of the RNA coupled with mass spectrometry analysis of bound proteins. From hundreds of potential hits, we have cross-validated a small subset of proteins that we suspect directly interact with BC200. We have recently discovered that the last 80 nucleotides of BC200 can be truncated in human cells, and that this truncation may be the key event regulating carcinogenesis. Our current hypothesis is that BC200 acts as a scaffold for a protein regulatory complex that interacts with messenger RNAs to regulate translation, with a different subset of proteins interacting with the RNA when truncated.

PROJECT:

The proposed research project will use a combination of biochemistry, structural biology, and molecular biology to characterize the direct interactions between BC200 and target proteins identified from our screen. Molecular biology approaches coupled with bacterial/eukaryotic expression systems will be used to produce the BC200 binding partners (starting with one initially and building to more as time permits). Expression/purification protocols will need to be individually developed for each protein. BC200 will be produced (using an established protocol) using *in vitro* transcription, as will the 80-nucleotide truncation. RNA-protein binding affinity and complex stability will be evaluated. Promising complexes will be structurally characterized using cryo-electron microscopy approaches.





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Project #24:
Understanding Fluorine NMR Chemical Shifts

Dr. Katie Mitchell-Koch (katie.mitchellkoch@UManitoba.ca, (204) 474-6053)

INTRODUCTION:

Fluorine NMR spectroscopy is a valuable tool for studies of small molecules, as well as protein structure-function through the incorporation of fluorinated amino acids. The fluorine nucleus is highly sensitive to environment and bonding, displaying a broad range of chemical shifts (~800 ppm). It is generally understood that multiple factors influence fluorine chemical shifts in proteins, including local dielectric environment, hydrogen bonds, and solvation waters. However, the scientific community does not have a framework for interpreting what, exactly, the nucleus is reporting on. Our goal is to address these drawbacks through computationally-assisted assignment, interpretation, and prediction of fluorine nuclear resonances in different environments.

PROJECT:

Our work will use computational methods, primarily density functional theory (DFT) calculations to calculate fluorine chemical shifts with different models. We will compare the calculations with published values of fluorine chemical shifts in molecules that have been studied by systematically varying electronic structure or solvent environment. The contributions of different orbitals to the ^{19}F chemical sfhits will be calculated using Natural Chemical Shielding Analysis, in order to understand the origins of differences in fluorine chemical shifts. We will also examine the influence of specific solvent interactions on fluorine chemical shifts in a series of fluorinated aromatic compounds.

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Project #25:
Toward Improved Non-Aqueous Biocatalysis:
Enzyme Structure-Dynamic in Ionic Liquids

Dr. Katie Mitchell-Koch (katie.mitchellkoch@UManitoba.ca, (204) 474-6053

INTRODUCTION:

Enzyme catalysis is an area for the development of green chemistry, offering mild conditions, atom efficiency, and reducing the use of harsh chemicals required for chemical transformations such as oxidation. Enzyme catalysis can be a crucial tool for the efficient production of commodity and fine chemicals from carbon precursors, including biomass. However, many organic compounds are sparsely soluble in water, the native solvent of enzymes. This can be overcome by the use of organic solvents and ionic liquids,[1] which solubilize hydrocarbons and expand enzyme function. Several lipases have been shown to retain their structure and catalytic function in organic solvents and ionic liquids. We have developed methods to simulate enzymes in organic solvent and ionic liquids.[2]

PROJECT:

Our work will use molecular dynamics simulations to model enzymes in newly-developed ionic liquids that are designed, synthesized, and characterized by our collaborators. We will characterize solvent-protein interactions in novel ionic liquids and monitor variations in enzyme structure and dynamics due to solvent.[3] Comparing results to experimental data from our collaborator, we will correlate simulations data with enzymatic activity to guide the design of new ionic liquids and biocatalysis strategies.

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3. Dahanayake, J. N.; Mitchell-Koch, K. R. “How Does Solvation Layer Mobility Affect Protein Structural Dynamics?” *Front. Mol. Biosci.,* 2018, *5:65*, 1-20.

Project #26:
Mapping the Protein Hydration Layer

Dr. Katie Mitchell-Koch (katie.mitchellkoch@UManitoba.ca, (204) 474-6053

INTRODUCTION:

The Mitchell-Koch group focuses on the solvation layer surrounding proteins, as these intimately-related molecules are integral to protein structure, dynamics, and function, yet are often ignored in drug design and studies of biomolecular function. At the protein surface, water molecules exhibit altered dynamics- namely, diffusion, reorientation, and hydrogen bond lifetimes. The extent to which the dynamical properties of water are altered relative to bulk water varies around different regions of the protein. Using computational methods, we can map the water dynamics regionally at the protein surface, and characterize how water molecules are arranged around the protein surface (*i.e.* describe the local water structure). We found previously that the structure and dynamics of water in the solvation layer is connected by an excess entropy relationship[1] and we continue to explore relationships among water structure & dynamics and protein structure & dynamics.

PROJECT:

Our work uses molecular dynamics simulations to simulate proteins in water, and then we carry out specialized analysis to characterize the solvation layer around the proteins. Systems to be studied include a series of homologous proteins, starting with alcohol dehydrogenases. Our work will compare properties of the hydration layer across these enzymes with similar function, to see to what extent the solvation layer properties are similar or different at regions of the protein with similar function (for example, at the cofactor binding cleft). Our data will contribute to the creation of a data set in which the relationship between protein structure and hydration layer properties can be examined.

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Project #27:
Design and development of protein reporters for CART-cell populations

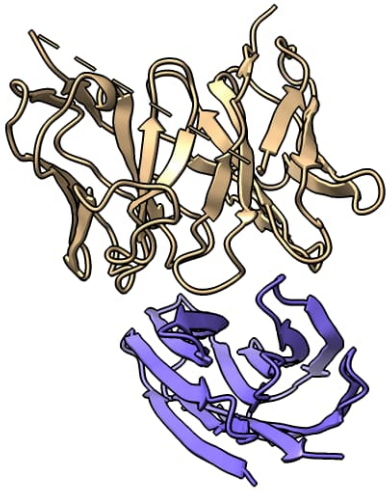
Dr. Zev Ripstein (Zev.Ripstein@UManitoba.ca, (204) 474-8504)

INTRODUCTION:

Induced pluripotent stem cells represent an emerging therapeutic technology with extensive applications in studying and treating autoimmune diseases and cancers. One major use is Chimeric Antigen Receptor (CAR) T-cell therapy which involves extracting blood samples from a patient through a procedure called leukapheresis, which collects lymphocytes, or white blood cells. By using T-cell engineering, scientists enhance the T-cell receptors in these white blood cell samples before reinfusing them into the patient. This process increases the recognition of antigens associated with B-cell cancers, aiding in their elimination.

PROJECT:

This project proposes the development of a novel CD19 mimic designed to bind to and report on the presence of chimeric antigen receptors (CARs) on T cells. The objective is to engineer a synthetic protein molecule that is stable, easily expressed and emulates the natural binding interaction of CD19 with its T-cell receptors, specifically targeting CARs incorporating CD19 co-stimulatory domains. The proposed CD19 mimic will be equipped with a detectable marker, allowing for real-time monitoring and quantification of CAR expression on the cell surface. This project aims to facilitate the assessment of CAR-T cell populations and their functional status, ultimately optimizing CAR-T cell therapies.



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Project #28:
Utilizing machine learning models to thermo-stabilize protein reagents

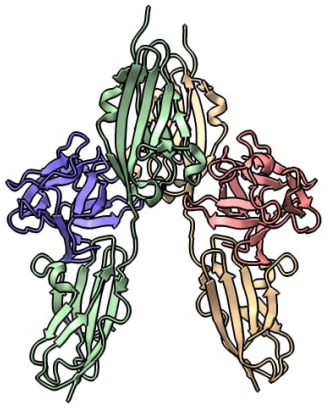
Dr. Zev Ripstein (Zev.Ripstein@UManitoba.ca, (204) 474-8504)

INTRODUCTION:

Induced pluripotent stem cells represent an emerging therapeutic technology with extensive applications in studying and treating autoimmune diseases and cancers. Culturing and propagating these pluripotent stem cells require various protein growth factors. One such factor, Basic Fibroblast Growth Factor (bFGF), is essential for maintaining stem cells in mammalian cell cultures but suffers from instability, with a short half-life of just 8 hours in culture media. This instability limits cell growth over extended periods, necessitating daily media changes, which are both costly and labor-intensive. Recent advancements in neural networks, which predict optimal protein sequences for specific protein folds, have enabled rapid in silico predictions of thermally stabilizing mutations applicable to a wide range of proteins.

PROJECT:

This project aims to design and test thermally stabilizing mutations for bFGF. The design phase will involve optimizing the bFGF sequence using a combination of sequence prediction tools and molecular dynamics simulations. The synthesized bFGF will then undergo thermal stability testing using biophysical and structural techniques, along with cell-based assays to assess functionality. The central hypothesis is that a stable bFGF protein will significantly extend its half-life in cell culture. Promising candidates will be evaluated for their ability to retain binding and signaling functions, with structural characterization performed using cryoEM.



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Project #29:
Substrate influence on the adsorption behavior of 2D materials

Dr. H. Georg Schreckenbach (schrecke@cc.umanitoba.ca, 204-474-6261)

INTRODUCTION:

The field of two-dimensional (2D) materials came into being with the discovery of graphene, the "chicken-wire molecule" [1]. The field has exploded since, and various other 2D materials have been synthesized or computationally predicted, spanning a large part of the periodic table. [2] One potential, promising application of novel 2D materials is sensing, such as of small organic molecules (Figure 2) [3] or of metals [4, 5]. This is based on the unique electronic response of the material upon adsorption [3]. While some 2D materials (e.g. graphene) have been synthesized as freestanding materials, most require a support. For instance, 2D SnTe (Figure 1) has been grown on SiC, mica, and graphene, among others. The presence and nature of a support will influence the electronic structure of the 2D material, and hence its adsorption and sensing behavior.

PROJECT:

In this project, we will use computational chemistry (density functional theory, DFT) to investigate the influence of substrates on the absorption behavior of prototypical 2D materials. As a first step, this requires building computational models of the 2D–substrate interface. Subsequently, these models will then be used to study small-molecule adsorption and, hence, sensing. The specific choice of systems [2D material(s), substrates, adsorbates] will be determined at a later stage.

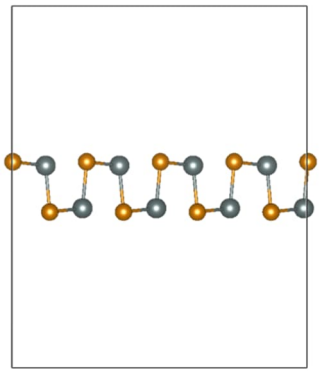

Figure 1. Side view of SnTe monolayer.

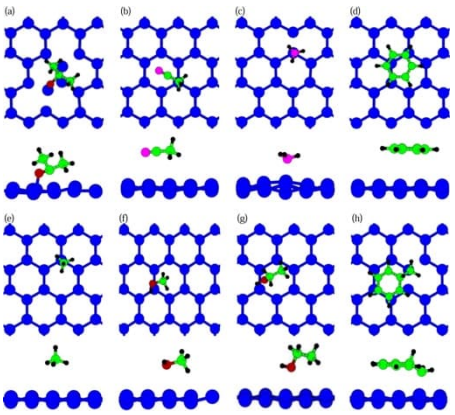

Figure 2. Computationally predicted silicene–adsorbate structures, top and side views. [3]

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Project #30:
Computational Actinium Chemistry

Dr. H. Georg Schreckenbach (schrecke@cc.umanitoba.ca, 204-474-6261)

INTRODUCTION:

"Theoretical actinide molecular science", quantum-chemical modeling of actinide complexes, is motivated by fundamental and practical considerations. [1] Fundamental interest arises because of the unique chemistry of these elements. For instance, it is only in this part of the periodic table that f-orbitals contribute significantly to bonding. A novel practical application comes with the proposal to apply the actinium isotope ^{225}Ac (half-life 10 days) as a radiotherapeutic agent for cancer treatment, particularly for difficult to treat late-stage cancers (Targeted Alpha Theraphy). [2, 3]

PROJECT:

The chemistry of actinium is not very well known [4] since all isotopes are highly radioactive, and the element occurs naturally only in trace amounts. (The most stable isotope, ^{227}Ac, has a half-life of about 22 years.) Therefore, it is the goal of the project *to use computational chemistry to fill in some of these knowledge gaps*. Actinium is quite intriguing chemically in that it behaves essentially as a transition metal but has empty 5f orbitals that are in principle available for bonding as well.

Following a recent study from our group [5] and using the known [2] Ac aquo complex as reference point, the project student will model complexes with various small, biologically relevant compounds (e.g. amino acids) as ligands. The project student will use these systems as model systems to further establish bonding patterns, addressing questions such as participation of f orbitals in bonding, the nature of bonds (covalent vs. ionic contributions), or the equatorial coordination number in solution (i.e. the number of bonds around actinium – this is particularly difficult to determine experimentally) and its relationship to bonding and thermodynamic stability. Thus, we will add to the knowledge of actinium chemistry, in relationship to that of its neighbors in the periodic table.

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Project #31:
Using Computational Chemistry to Predict the Properties of Biphenanthridines: New Frontiers

Dr. H. Georg Schreckenbach (schrecke@cc.umanitoba.ca, 204-474-6261)

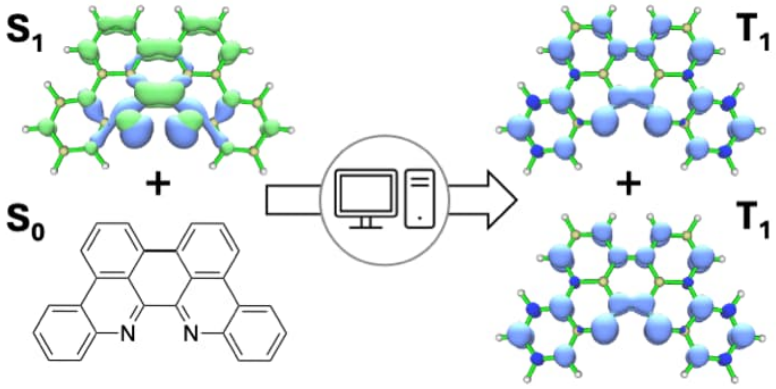
Dr. David E. Herbert (david.herbert@umanitoba.ca, 204-474-7535)

INTRODUCTION:

Aromatic compounds in general, and substituted aromatics such as *N*-heterocycles in particular, are of great interest for applications from medicines to materials. One prominent example is as "singlet fission materials" which can effectively double the current obtainable from solar energy harvesting.[1] Recently, the Herbert group has developed synthetic methods to coupled benzannulated *N*-heterocycles such as "biphe" (6,6'-biphenanthridine).[2] Collaborative work between the Schreckenbach and Herbert groups have subsequently used computational methodologies developed here at UM[3] to computationally screen biphe analogs for use as singlet fission materials, leading to a peer-reviewed publication based on the results from a past 4710 project.[4]

PROJECT:

The goal of this project is to extend this protocol using computational chemistry to predict the structural and optical properties of biphe and its analogs, as both neutral complexes and in their (di)anionic forms. The interested student would work primarily in the Schreckenbach group, but in close contact with the Herbert group, to simulate the absorption spectra of these compounds and evaluate their lowest lying singlet and triplet state structures and energies for potential application in singlet fission and related applications.



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[2] D.B. Nemez, I.B. Lozada, J.D. Braun, J.A.G. Williams, D.E. Herbert *Inorg. Chem.* 2022, *61*, 13386-13398

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Project #32:
Design, synthesis and biological properties of amphiphilic aminoglycosides:
Rescuing antibiotics from resistance against Gram-negative pathogens

Dr. Frank Schweizer (Frank.Schweizer@umanitoba.ca, 204 474 7012) Supervisor

INTRODUCTION:

Antimicrobial resistance is one of the largest threats to public health and economic growth <1>. Despite significant investments into antibiotic discovery in the past, no new antibiotic class against Gram-negative bacteria (GNB) has been approved in half a century. The reasons for this failure are due to low outer membrane (OM) permeability and extensive efflux generally referred to as the "Achilles Heel" in antibacterial drug discovery (FIG. 1) <2>. To overcome this bottleneck, the project plans to develop amphiphilic aminoglycosides with little or no antibacterial activity that will enhance OM permeability and/or reduce efflux of antibiotics in GNB <3>.

PROJECT:

The project will involve the synthesis of unnatural, amphiphilic aminoglycosides derived from the aminoglycoside sisomycin. Organic chemistry will be used to prepare a small library of amphiphilic sisomycin analogs. All analogs will be purified by reverse phase chromatography and characterized by NMR. Subsequently, the synthesized compounds will be evaluated for their effects on OM permeability and efflux of clinically approved antibiotics against clinical isolates of multidrug-resistant Gram-negative pathogens. Synergy of the compounds in combination with antibiotics will be determined followed by time/kill studies. Hit compounds which enhance OM permeability and/or reduce efflux of antibiotics will be assessed for potential cytotoxicity against human cell lines.

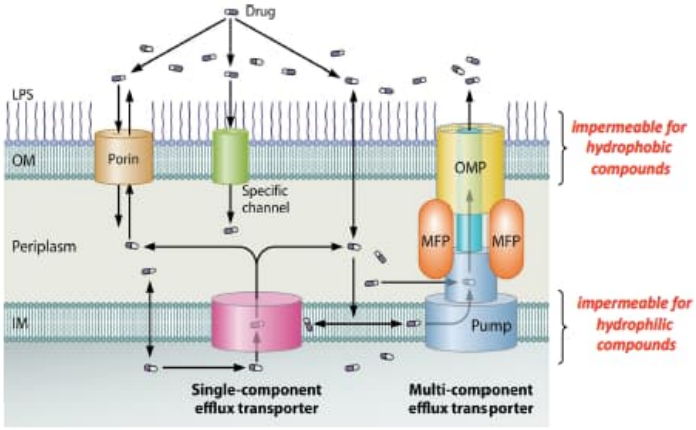

Fig. 1

REFERENCES:

<1> taken from the Lancet https://doi.org/10.1016/S0140-6736(21)02724-0 , January 20, 2022

<2> *Nature.* 2016, *529*, 336-343.

<3> *Clin. Microbiol. Rev.* 2018, *2*, 2018, e00077-17

Project #33:
Design, synthesis and biological properties of novel polymyxins:
Rescuing antibiotics from resistance against Gram-negative pathogens

Dr. Frank Schweizer (Frank.Schweizer@umanitoba.ca, 204 474 7012) Supervisor

INTRODUCTION:

Antimicrobial resistance is one of the largest threats to public health and economic growth <1>. Despite significant investments into antibiotic discovery in the past, no new antibiotic class against Gram-negative bacteria (GNB) has been approved in half a century. The reasons for this failure are due to low outer membrane (OM) permeability and extensive efflux generally referred to as the "Achilles Heel" in antibacterial drug discovery (FIG. 1) <2>. To overcome this bottleneck, the project plans to develop novel polymyxin analogs with little or no antibacterial activity that will enhance OM permeability and/or reduce efflux of antibiotics in GNB <3>.

PROJECT:

The project will involve the synthesis of unnatural, amphiphilic polymyxin analogs using solid phase peptide chemistry. Organic chemistry will be used to prepare a small library of polymyxin analogs. All analogs will be purified by reverse phase chromatography and characterized by NMR. Subsequently, the synthesized compounds will be evaluated for their effects on OM permeability and efflux of approved antibiotics against clinical isolates of multidrug-resistant Gram-negative pathogens. Synergy of the compounds in combination with antibiotics will be determined followed by time/kill studies. Hit compounds which enhance OM permeability and/or reduce efflux of antibiotics will be assessed for potential cytotoxicity against human cell lines.

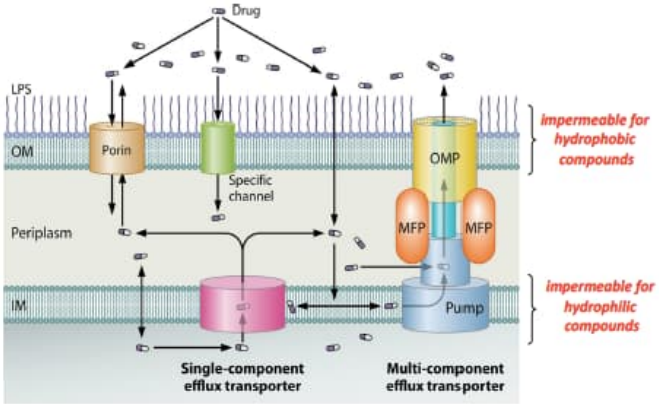

Fig. 1

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<2> *Nature.* 2016, *529*, 336-343.

<3> *Clin. Microbiol. Rev.* 2018, *2*, 2018, e00077-17

Project #34:
Maternal Offloading of Polycyclic Aromatic Compounds in Seabirds

Dr. Gregg Tomy (Gregg.tomy@UManitoba.ca, (204) 474-8127)

INTRODUCTION:

Polycyclic aromatic compounds (PACs) are a complex class of compounds that are the main constituent of crude oils. In addition to their pyrogenic origins, PACs can also be formed naturally by the incomplete combustion of organic matter. These compounds have been detected in every environmental compartment including air, water, soil/sediment and biota. Because of their high trophic position, seabirds (specially seabird eggs) are used extensively as a media to monitor the fate and behaviour of these PACs in the environment.

PROJECT:

Maternal transfer of persistent organic pollutants from mother to offspring has been shown for compounds like polychlorinated biphenyls and polybrominated diphenyl ethers. However, relatively little is known about the maternal offloading of PACs. Here we use paired maternal seabird liver and eggs and examine the concentrations of PACs in both tissue types. The experimental workflow will be extracting PACs from liver and eggs using accelerated solvent extraction and microbead beating extraction, respectively. Detection and quantitation of PACs will be done using gas chromatography tandem mass spectrometry. Results of this study will provide new information on the extent of maternal transfer of PACs in seabirds and what PAC-types are more easily transfer from mother to offspring.

Project #35:
Crammed Carbon Cages

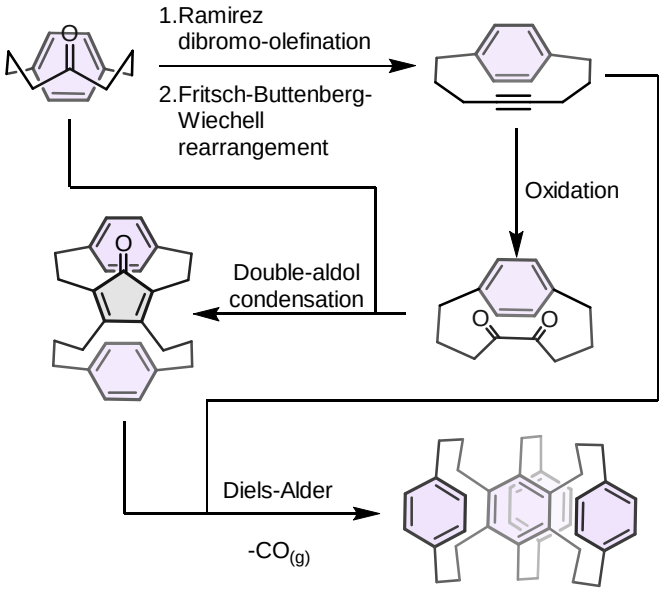
Dr. Joshua Walsh (Joshua.Walsh@UManitoba.ca, (204) 474 6605)

INTRODUCTION:

Cyclophanes have attracted the attention of organic chemists for more than 70 years.[1][2] Cyclophane research over the past decades has focused on aromatic-aromatic interactions[3] and contesting the textbook definition of aromaticity.[4] Close contacts of aromatic surfaces with isolated functional groups have been overlooked. This gap is a result of the current state of the art in cyclophane synthesis which has remained nearly unchanged since its early days. Recently, the Walsh lab has developed a convenient method to synthesize bridge-functionalized cyclophanes and in this project, we aim to put that methodology to good use.

PROJECT:

This project is focussed on utilizing our new synthetic methodology to access cyclophanes through a short sequence of reactions. This will allow us to answer fundamental questions about what happens when antiaromatic systems are crammed into the ring current of aromatics as well as allowing the exploration of the chemical space that is opened when bridge-functionalized cyclophanes move from being the end of the synthetic road, to the starting point for more complex structures. The student involved in this project will be mainly involved in organic synthesis as well as characterization including NMR, mass spectrometry, FT-IR, UV-vis and fluorescence spectroscopy.



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Project #36:
Synthesis of Soft Chromophores for Singlet Fission

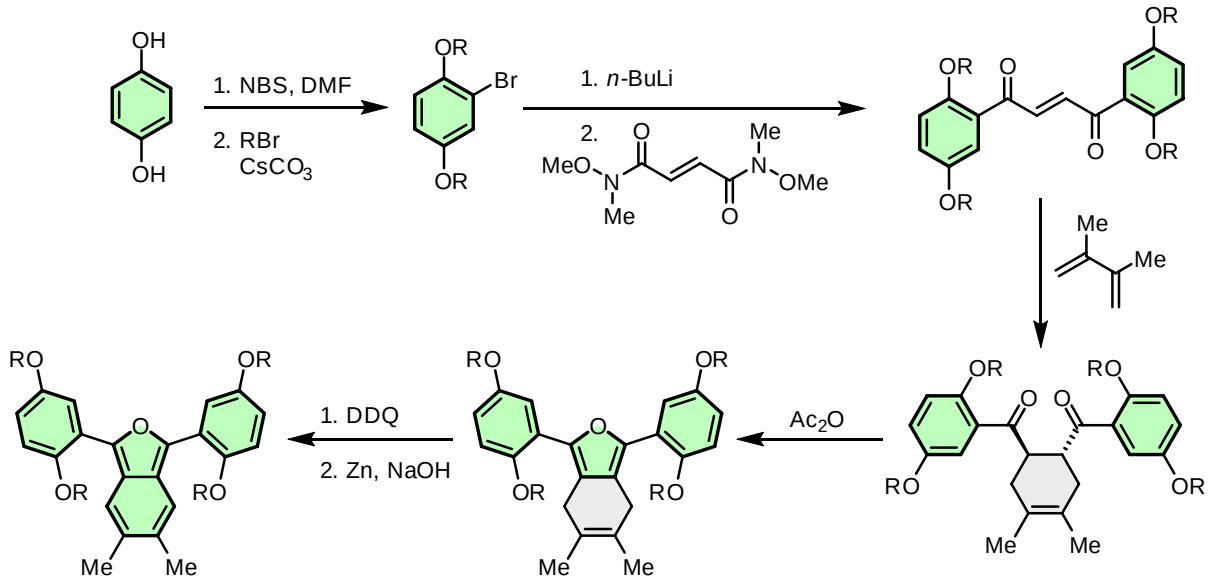
Dr. Joshua Walsh (Joshua.Walsh@UManitoba.ca, (204) 474 6605)

INTRODUCTION:

Singlet fission (SF) is a spin-allowed photophysical phenomenon that holds the potential to surpass the upper limit in solar cell efficiency, known as the Shockley-Queisser limit.[1] Through the conversion of a singlet excited state to two triplet excited states, SF can generate two lower-energy excitons from a single photon, thereby mitigating some thermal losses. While SF has been observed in diphenylisobenzofuran, the compound suffers from low stability under irradiation and presents challenges in characterization due to its multiple thin-film morphologies.[2]

PROJECT:

This project aims to address the limitations of diphenylisobenzofuran by synthesizing room-temperature isotropic liquid (RTIL) derivatives. Liquefaction is expected to yield materials that are highly processable and photostable, with the isotropic nature mitigating morphological issues. Sterically demanding alkyl chains will be introduced to the planar core to render the chromophore an RTIL. [3] The potential of these derivatives for use as singlet fission dyes will be investigated. The student involved in this project will primarily engage in organic synthesis and characterization techniques, including NMR, mass spectrometry, FT-IR, UV-vis, and fluorescence spectroscopy.



REFERENCES:

1. A. Rao, R. H. Friend *Nat. Rev. Mater.* 2017, *2*, 17063.

2. J. L. Ryerson et al. *J. Phys. Chem. C* 2014, *118*, 12121.

3. F. Lu et al. *Sci. Rep.* 2017, *7*, 3416.

Project #37:
From URL to IRL: Making Theoretical Predictions Come True!

Dr. Joshua Walsh (joshua.walsh@umanitoba.ca, 204-474-6605)

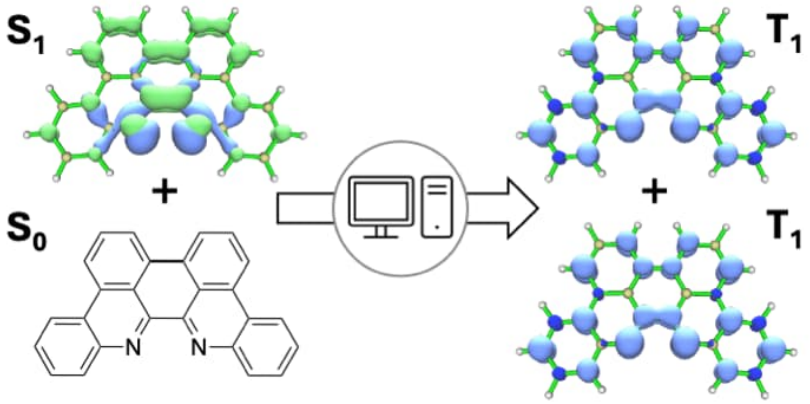
Dr. David E. Herbert (david.herbert@umanitoba.ca, 204-474-7535)

INTRODUCTION:

Aromatic compounds in general, and substituted aromatics such as *N*-heterocycles in particular, are of great interest for applications from medicines to materials. Recently, the Herbert group has developed synthetic methods to coupled benzannulated *N*-heterocycles such as “biphe” (6,6’-biphenanthridine).[1] Computational screening revealed biphe analogs show promised as singlet fission materials.[2] “Singlet fission materials” can effectively double the current obtainable from solar energy harvesting.[3]

PROJECT:

The goal of this project is to *experimentally* realize some of the structures dreamed up in our prior computational work and to confirm their predicted structural and optical properties. The Walsh group has expertise in the *functionalization* of extended aromatic structures.[4] The interested student would work closely with both groups to prepare a range of analogs of biphe and examine their photophysical properties to help make our chemical dreams come true!



REFERENCES:

[1] D.B. Nemez, I.B. Lozada, J.D. Braun, J.A.G. Williams, D.E. Herbert *Inorg. Chem.* 2022, *61*, 13386-13398

[2] K.A. Veilleux, G. Schreckenbach, D.E. Herbert *Mol. Sys. Des. Eng.* 2024, *9*, 423-435

[3] M. Smith, J. Michl *Chem. Rev.* 2010, *110*, 6891-6936

[4] J. C. Walsh, K. M. Williams, D. Lungerich, G. J. Bodwell, *Eur. J. Org. Chem.* 2016, *36*, 5933–5936

6. Appendix A

Signature Sheet for Student – Faculty Interviews

Student: _____ _____
(print name) (student #)

e-mail: _____
(University of Manitoba e-mail address)

Program: _____ _____
(e.g Honours Chemistry) (year in program on Sep. 6, 2024)

Interview #1:

Faculty member: _____
(print name)

_____ _____
(signature) (date)

Interview #2:

Faculty member: _____
(print name)

_____ _____
(signature) (date)

Interview #3:

Faculty member: _____
(print name)

_____ _____
(signature) (date)

Notes:
1. Each student should interview at least 3 faculty members willing to offer CHEM4710 projects. During the meeting the nature of the project should be explored and expectations of the student and advisor should be discussed. You can interview as many faculty members as you wish.

2. Students should prioritize their project choices, a minimum of 3 projects are required. Note that every student can apply for any project. Students are strongly discouraged from only choosing projects from a single advisor.

7. Appendix B

Student Project Choices

Student: _____ _____
(print student name) (student #)

_____ _____
(student signature) (date)

Project choices (1 = highest priority, 2, 3,...)

Choice 1: Project title: _____ Project #____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 2: Project title: _____ Project #____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 3: Project title: _____ Project #____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 4: Project title: _____ Project #____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Choice 5: Project title: _____ Project #____

Supervisor: _____

I, the student, have carried out research with this research group before. YES___ NO___

Student comments:

8. Appendix C

CHEM 4710 - Research Project in Chemistry or Biochemistry - 2024/25

Course Coordinators:	Mario Bieringer
Office:	520c Parker Building
Email:	Mario.Bieringer@UManitoba.ca
Phone:	204-474-6258

Student - Advisor Agreement

This agreement is between

1. _____

a student registered in CHEM 4710 "Research Project in Chemistry or Biochemistry", hereafter called "the Student"

2. _____

a professor at the University of Manitoba, and an advisor of a CHEM 4710 student, hereafter called "the Advisor"

The Student agrees to carry out a research project, as described in the attached research proposal, under the direction of the Advisor. The student agrees to meet the goals and expectations that have been set out by the advisor. These goals and expectations will include not only the scientific aims of the project, but also the time commitment that is required of the student to achieve these goals. The student agrees to a schedule of attendance at regular meetings with the advisor and the research group. The student is expected to become an active member of the research group and will assume responsibility for maintaining a safe work environment in the laboratory. The student may also be expected to assume various duties in addition to those directly associated with the project in order to maintain the safe laboratory environment. The student understands that the main goal of the Research Project is to gain experience in the process of scientific research and that effort is evaluated as much as obtaining research results. The student agrees to meet the deadlines for reporting for both written reports and the oral presentation as set out in the course outline.

The Advisor pledges to support the student in the research project by making available to the student the full resources of the research group and department. In addition the advisor will provide the scientific and intellectual guidance to ensure the success of the project. The advisor agrees to hold regular meetings with the student to discuss the current progress and results. The advisor will encourage the student to develop skills in critical thinking and help to develop a sense of scientific independence. The advisor will provide the necessary training in lab techniques and ensure that the student has received adequate safety training relating to the project. The advisor will also provide the student with timely advice on the content and style of both written reports and oral presentations. The advisor also agrees to give the student appropriate credit for the results generated during the project. This may also include authorship on publications that are generated from the results of the project.

The Student:	The Advisor:
_____	_____
Date:	Date:_____

Please sign this form and submit to the course co-ordinator by September 20th, 2024.