4th-Year Chemistry Thesis Projects 2021-2022 Academic Year

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Application for Thesis Information and Instructions

NOTE re Coronavirus Lockdown: Due to the disruptions caused by the Campus closure,

while it is currently assumed that lab work will be able to resume in Sept 2021, the Honours thesis projects may be subject to postponement from an extended closure and/or changes to accommodate future restrictions related to the Coronvirus outbreak.

Introduction

The thesis option consists of two courses: CHEM 4410U and CHEM 4420U. Each course constitutes 3 credit hours of the 120 credit hours required for an honours degree. Students are expected to enroll and pass CHEM 4420U immediately following CHEM 4410U. Under most circumstances, these courses will be taken in the fall and winter semesters of the student's final academic year.

The completion of the honours thesis is expected to require at least 230 hours of work on the part of the student (i.e., an average of 9 hours per week in each of the two semesters). The majority of this time will be spent in the laboratory conducting original research under the supervision of a faculty member. The evaluation of the chemistry honours thesis will be based on three components: i) in-lab performance; ii) oral defence of the thesis; iii) written dissertation. Both the student and the faculty supervisor should familiarize themselves with policies and procedures governing the honours thesis. These guidelines should not be interpreted as superseding any regulations described in the university calendar or general policies of the Faculty of Science.

Qualification for the Honours Thesis

To qualify for the honours thesis in chemistry a student must:

1. Have completed 90 credit hours toward their degree by the beginning of the fall semester of the year in which they intend to take CHEM 4410U / 4420U.
2. Have a GPA of 2.0 and be in clear academic standing.
3. Have passed at least four of: CHEM 3040U, CHEM 3120U, CHEM 3220U, CHEM 3520U and CHEM 3540U.

Students who have not completed 90 credit hours at the end of their third-year may be admitted provisionally to CHEM 4410U if they can show that they will have completed 90 credit hours by the start of the fall semester.

Selection of a Project

Each year faculty members in the Faculty of Science willing to supervise undergraduate theses in chemistry will provide a list of thesis projects from which a student may choose. Normally, a student completing a program in chemistry will do a project under

the supervision of one of the chemistry faculty members. However, projects from other disciplines (or even other Faculties) may also be acceptable as long as the research involves significant chemistry content. Such projects require the approval of the Chemistry Undergraduate Studies Committee.

Students may apply to work on a project by completing the “Honours Thesis Application” form available on the Faculty of Science website. The completed form is submitted by email to the current Undergraduate Program Director (UPD) for Chemistry (Fedor.Naumkin@uoit.ca in 2021). Acceptance by an individual supervisor is not guaranteed and is at the sole discretion of the supervisor. Students must apply to work on a project by **April 30** of the year prior to starting the research project. The UPD will inform students asap (by May 31st at the latest) if they have been selected by a supervisor and are approved to register in CHEM 4410U/4420U.

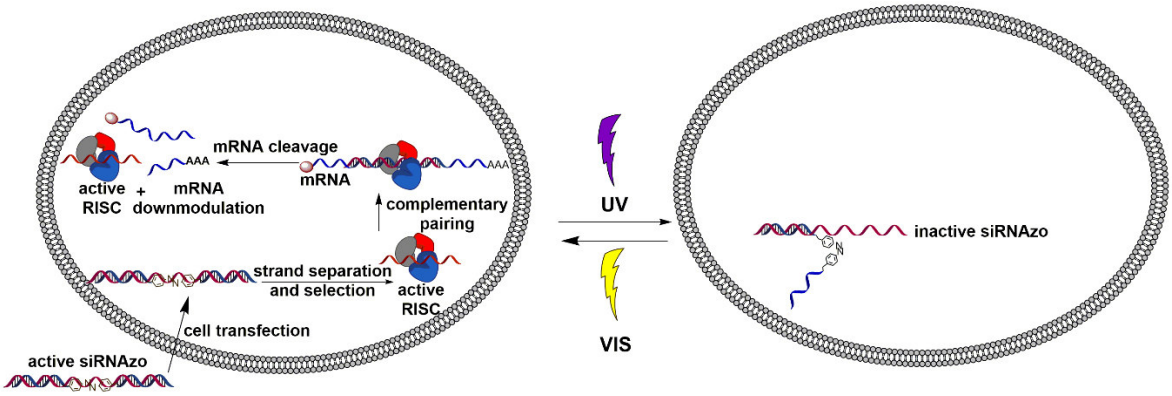
Professor Jean-Paul Desaulniers, Professor – Research Profile

The Desaulniers research group in Chemical Biology uses tools of organic chemistry, biochemistry, biophysical chemistry, and molecular biology to target, probe, and understand various components of gene expression. Organic chemistry is a powerful research tool for biology, because it allows us to answer key questions of biological importance. Diverse projects in our group range from the use of synthetic organic chemistry to generate new molecules with potential beneficial properties, to cell-based biological characterization of macromolecular-ligand interactions.

Research Projects for Chemistry Students for the 2021-2022 Academic Year

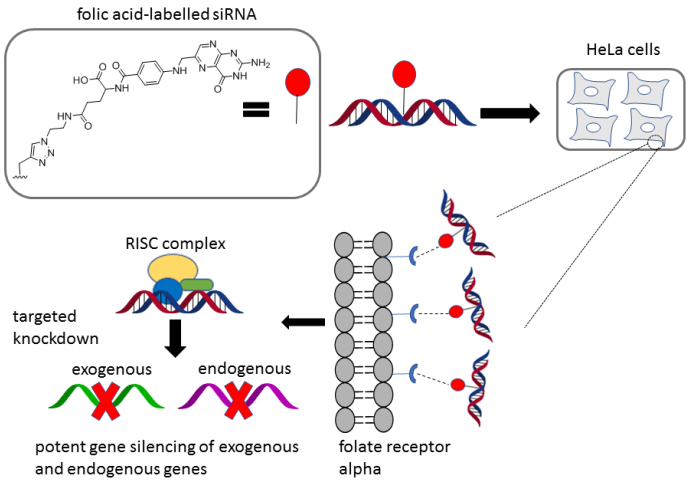
Project 1. Chemical Synthesis of Photoswitchable siRNAs

In this project, an undergraduate exchange student will work closely with a senior PhD student aimed at synthesizing new types of chemically-modified short-interfering RNAs that have photoresponsive properties. Through the use of organic chemistry, the student will synthesize phosphoramidite building blocks, and synthesize RNAs on solid-phase resin. This multi-disciplinary project will expose the exchange student to wide range of experimental techniques in a state-of-the art laboratory.



Project 2. Synthesis of Folic-Acid Derivative Phosphoramidites for Nucleic Acids

Recently, we have identified that folic-acid tagged siRNAs are excellent vectors for delivery of siRNAs into cells. To improve the synthetic utility of the chemistry, we are investigating the synthesis of folic acid phosphoramidites, that could allow for facile site-specific incorporation into a library of oligonucleotides. The student working on this project will be exposed to organic chemistry, and solid-phase synthesis.



Selected Publications (students bolded)

1) **L. Salim**, E. Goss, and J.-P. Desaulniers. "Synthesis and Evaluation of Modified siRNA Molecules Containing a Novel Glucose Derivative" *RSC Advances* **2021**, *11*, 9285-9289.

2) **L. Salim** and J.-P. Desaulniers. "To Conjugate or to Package? A Look at Targeted siRNA Delivery via Folate Receptors" *Nucleic Acid Ther.* **2021**, *31*, 21-38.

3) **M. L. Hammill**, G. Islam, and J.-P. Desaulniers. "Reversible Control of RNA Interference by siRNAzos" *Org. Biomol. Chem.* **2020**, *18*, 41-46.

4) **L. Salim**, G. Islam, and J.-P. Desaulniers. "Targeted Delivery and Enhanced Gene-Silencing Activity of Centrally-Modified Folic Acid-siRNA Conjugates" *Nucleic Acids Res.* **2020**, *48*, 75-85.

5) **K. Tsubaki**, **M. L. Hammill**, **A. J. Varley**, M. Kitamura, T. Okauchi, and J.-P. Desaulniers. "Synthesis and Evaluation of Neutral Phosphate Triester Backbone-Modified siRNAs" *ACS Med. Chem. Lett.* **2020**, *11*, 1457-1462.

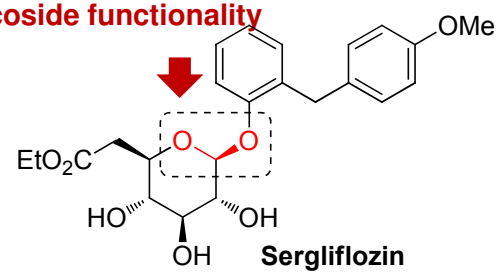
More information: Visit http://jpdesaulniers.com and check us out on Twitter (@JP_Desaulniers and @DesaulniersLab).

Dr. Yuri Bolshan

Associate Professor

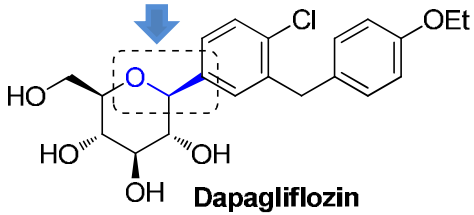
Pharmaceutical/Synthetic Organic Chemistry
Science Building, Room 4070

Natural but unstable
***O*-glycoside functionality**



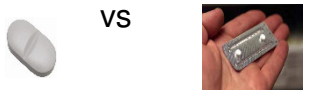
Sergliflozin

Unnatural and stable
***C*-glycoside functionality**



Dapagliflozin

Increased chemical and metabolic stability



Intravenous vs Oral therapy

OUR RESEARCH

Development of methodologies for the synthesis of unnatural *C*-glycosides and β–and γ-amino acids

Incorporation into anticancer drugs to improve their pharmacological properties. Emphasis: antileukemic drugs

γ-amino acids are known neurotransmitters Emphasis: Huntington's disease Parkinson's disease, pain

Synthesis of inhibitors for epigenetic proteins that modify DNA and control genes' expression

β–amino acids are metabolically more stable than α-amino acids Emphasis: synthetic analogs of natural antibiotics

Dr. Yuri Bolshan

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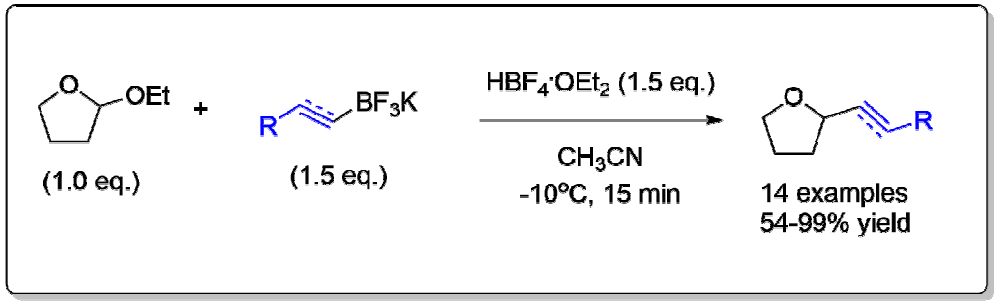
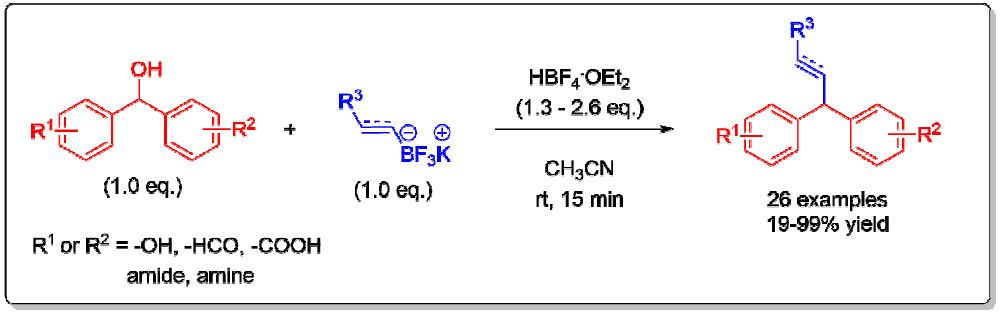
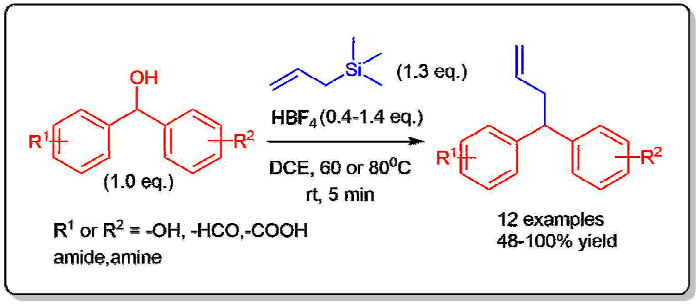
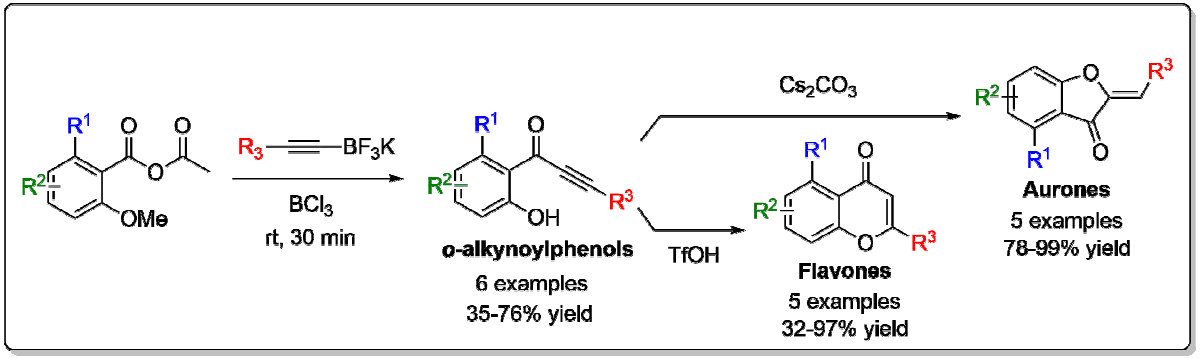


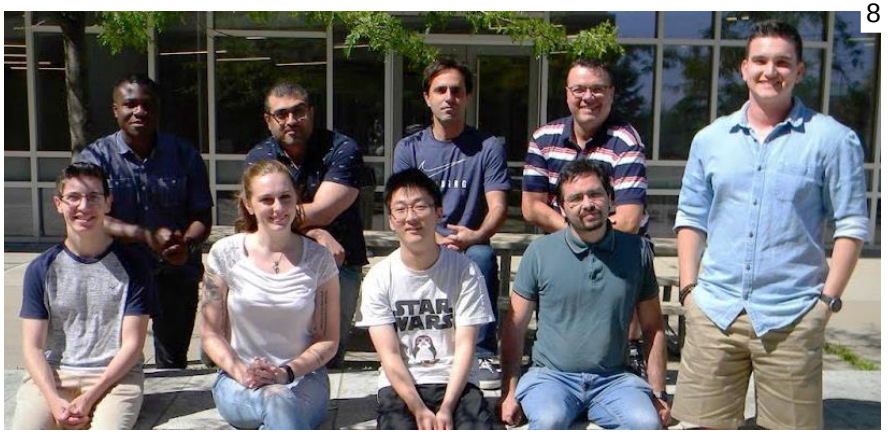




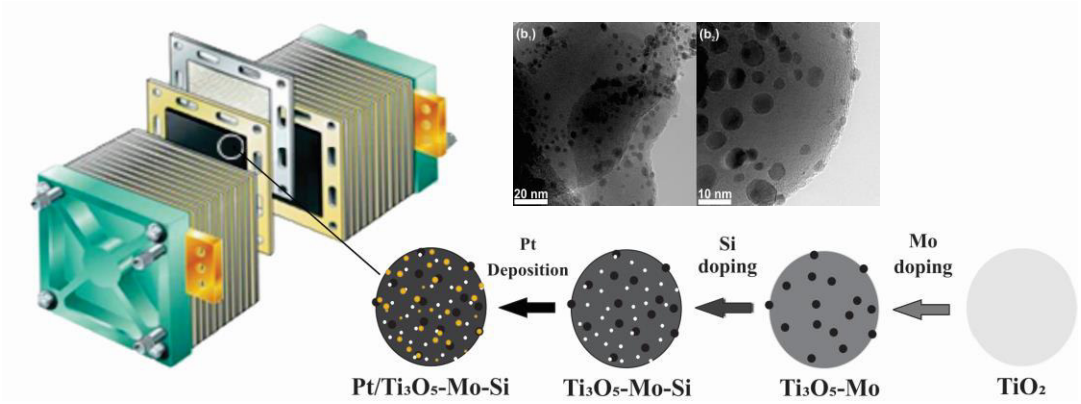


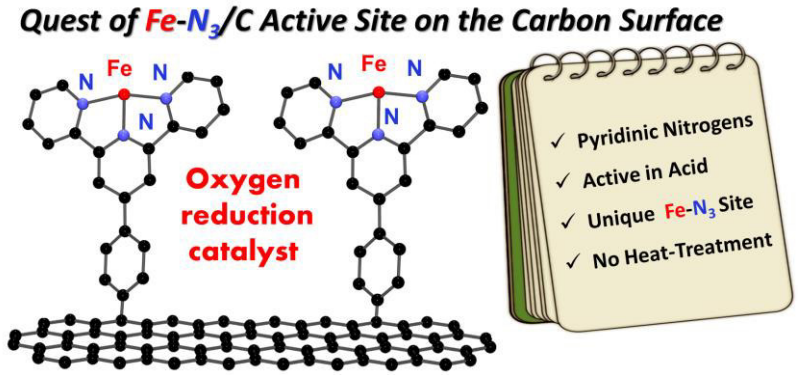
Dr. Brad Easton

Professor (Chemistry)
Ontario Tech Research Excellence Chair in Electrochemical Energy Materials
http://www.bradeaston.ca/



Research Interests: electrochemistry, materials chemistry, fuel cells, sensors, carbon surface chemistry, H_2 production





Selected publications based on undergraduate thesis:

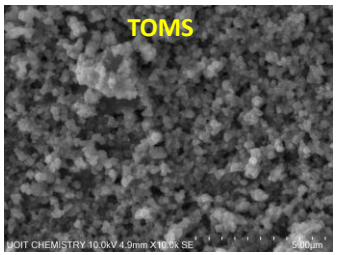
- **J. Poisson, H.L. Geoffrey,** I.I. Ebralidze, N.O. Laschuk, J.T.S. Allan, A. Deckert, E.B. Easton, O.V. Zenkina, J. Phys. Chem C., 122 (2018) 3419 – 3427.
- **K. M. Yarrow**, N. E. De Almeida, E. B. Easton, "The impact of pre-swelling on the stability of Nafion/SS composite membranes", *J. Therm. Anal. Calorim.*, 119 (2015) 807 - 814.
- **O. Reid**, F. S. Saleh, E. B. Easton, "Determining electrochemically active surface area in PEM fuel cell electrodes with electrochemical impedance spectroscopy and its application to catalyst durability", Electrochimica Acta, 114 (2013) 278 – 284.

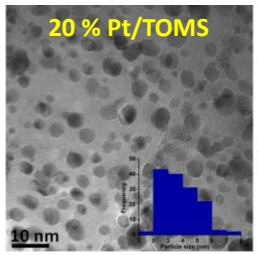
Dr. Brad Easton

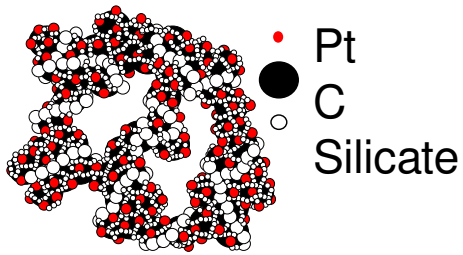
Professor (Chemistry)
Ph.D. (Memorial University of Newfoundland)
http://www.bradeaston.ca/

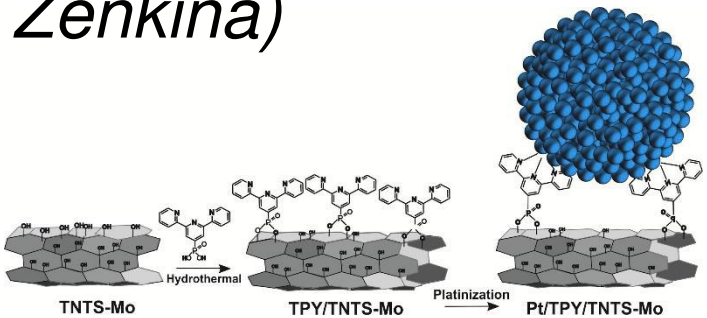
Available thesis projects for 2021/22

1. *Electrochemical stability of novel metal oxide-based fuel cell supports*
2. *Support effects related to photo-enhanced electro-oxidation of organic fuels*
3. *The preparation of coordination based functional electrochromic materials and metal wires on conductive surfaces. (co-supervised with Dr. Zenkina)*









Dr. Fedor Naumkin

Associate Professor of Chemistry

Ph.D. (General Phys. Inst., Russ. Acad. Sci.)

Research profile

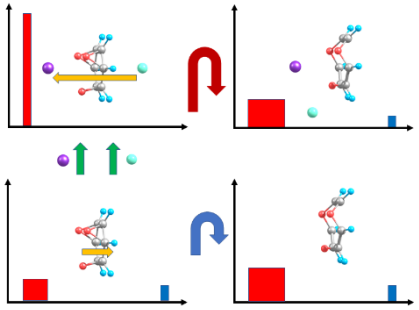
The Computational Nanochemistry research deals with the design of new nanosystems (clusters, intermolecular complexes, molecular junctions & interfaces), prediction and analysis of their structures, properties, and their inter-relationships. Of specific current interest are novel systems with molecules:

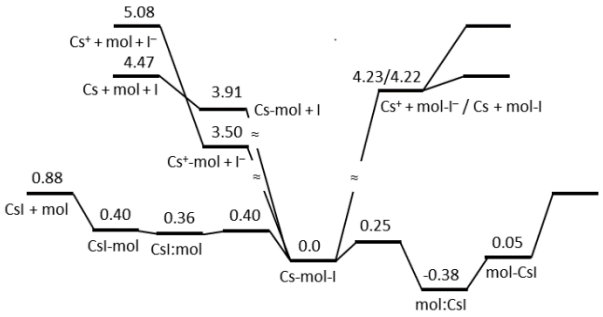
(1) trapped between counter-ions and stimulated to isomerise/react;

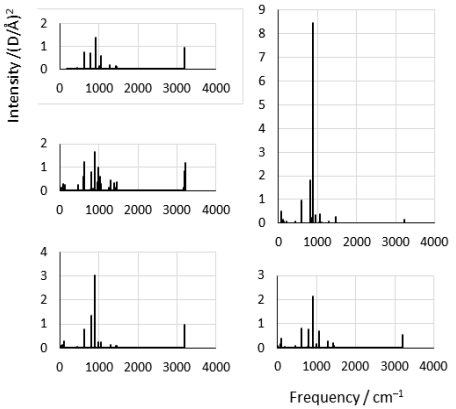
(2) linked by metals in assemblies with controllable shape alterations.

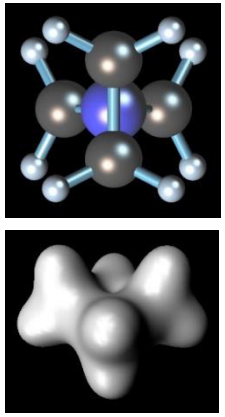
Various possible applications include:

- building blocks for materials with desired properties,
- light detection and utilization, molecular electronics and machinery,
- efficient energy storage at molecular level,
- molecular self-assembly and induced reactions, etc.









Dr. Fedor Naumkin **Contact: Fedor.Naumkin@uoit.ca**

- ***Project 1. Modelling of highly polar supramolecular species with enhanced IR activity and self-assembly capability.***
- ***Project 2. Evaluation of field-induced reactions of molecules trapped between counter-ions.***

The student will computationally investigate a series of insertion complexes of molecules trapped in counter-ion pairs.

These systems are to be suitably designed, their structures optimized in terms of energy, stability, polarity, IR spectra and other properties studied.

Project 1 focusses on the polarity and IR spectra, enhanced and system-structure sensitive. Dimerization as 1st step in self-assembly may also be involved.

Project 2 concentrates on the reaction barriers evolution inside the complex due to the mechanical pressure and electric field of the ions. A hyper-valence case may be included.

In either project the student will acquire practical experience of working with a state-of-the-art quantum-chemistry software and modern visualization tools, on high-performance computing facilities accessible at and through the UOIT.

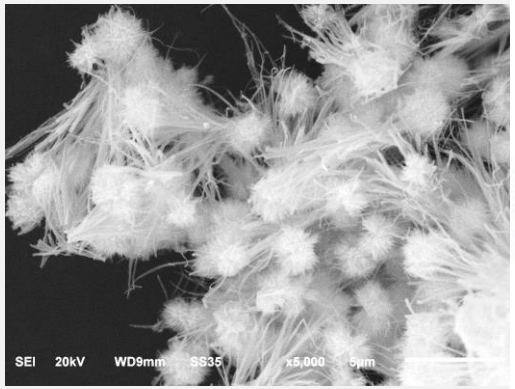
Selected publications (* marks students):

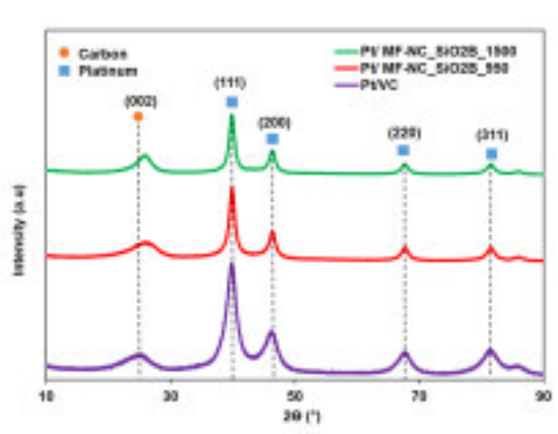
- S. Kerr* and F. Y. Naumkin, Field-assisted isomerization of a molecule intra-complexed with a counterion-pair, tracked via IR spectra. *To be submitted* (2021).
- M. Sullivan* and F. Y. Naumkin, Supramolecular complexes with insertion-enhanced polarity and tuned IR spectra. *Int. J. Quantum Chem*., 121, e26534 (2021).
- M. Sullivan* and F. Y. Naumkin, Highly polar insertion complexes with focused IR spectra and internal field-inhibited isomerization. *ChemPlusChem*, 85, 2438-45 (2020).

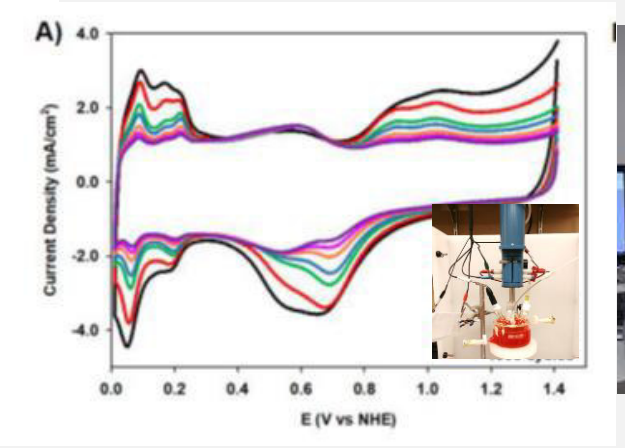
Professor Liliana Trevani, Associate Professor
Researcher Profile and Group Interests

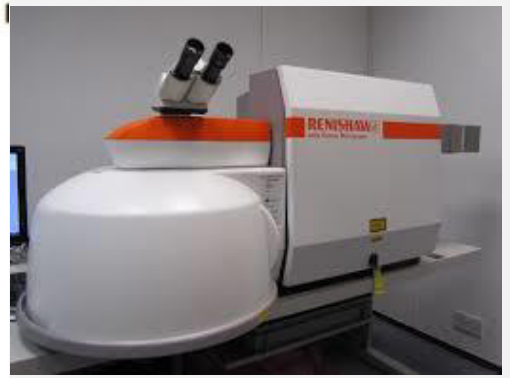
Research interests in our group involve: energy storage and conversion, hydrogen production, chemical sensors, nanomaterials, and hydrothermal systems.

Previous Honours Thesis projects in Trevani's group involved: physical chemistry studies aimed to investigate the formation of reaction by-products in the production of hydrogen using a thermochemical cycle, the development of mesoporous carbon catalyst support for polymer electrolyte membrane fuel cells using soft- and hard-template methods, the sol-gel synthesis of metal oxide composite aerogels/xerogels using solvothermal and supercritical carbon dioxide approaches, and synthesis of Au and Ag nanoparticles for surface-enhanced Raman spectroscopy.









Honours Thesis Projects in Trevani's Group for 2021-2022

- **Development of sensitive and selective chemical sensors based on copper, gold and silver nanostructures.**

This project will involve preparing microfluidic paper-based sensors using copper, gold, and silver functionalized nanoparticles. The student will explore different synthetic approaches for preparing the sensing nanomaterials and the design of the microfluid devices that will be used to detect and quantify species in solution using Raman and UV-visible spectroscopy. The project will be carried out in collaboration with Prof. MacDonald (FEAS) and Prof. Agarwal (Physics-FS). For additional information: Mahmud et al., Analyst, 141, 6446, 2016.

- **Construction and evaluation of an electrochemical Raman cell for studies in solution.**

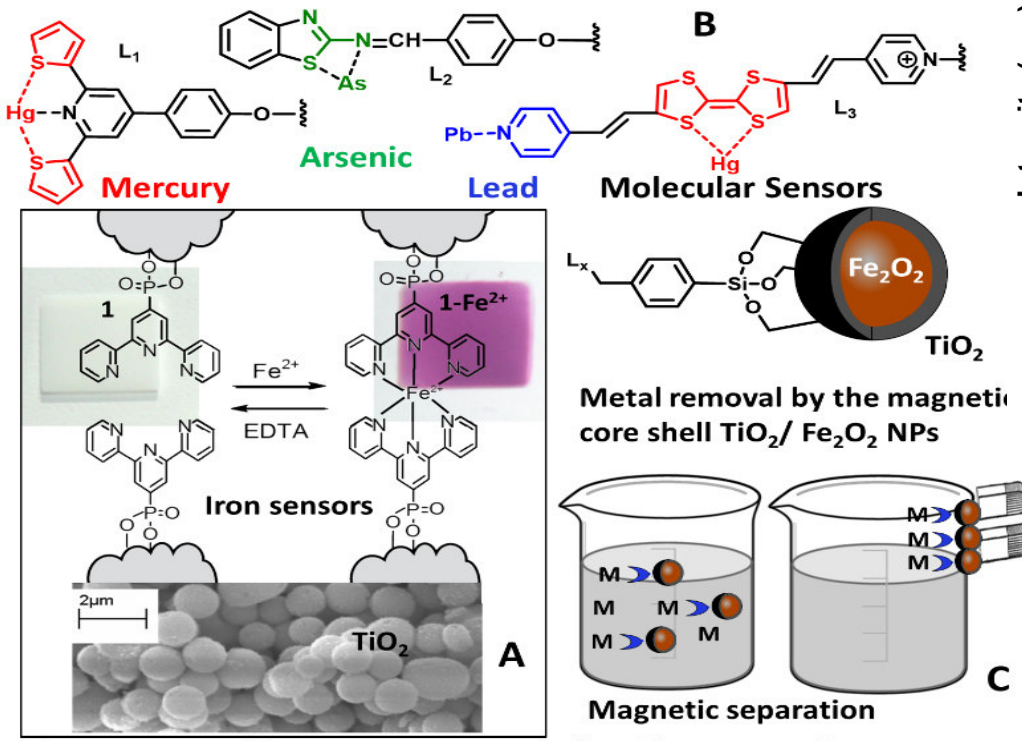
The project will contribute to developing an electrochemical Raman cell. The system will be used to perform materials characterization studies and identify and quantify species in solution. For additional information: Lynk et al., Anal. Chem. 90, 21, 12639-12646, 2018; Sasidharanpillai et al., J.Phys.Chem. B 123, (24), 5147-5159, 2020.

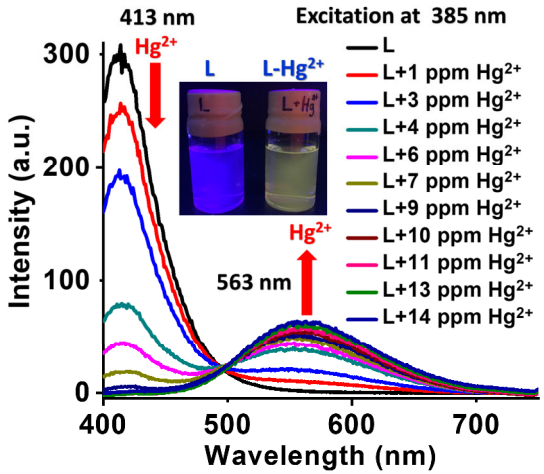
- **Carbon-based materials for sustainable energy**

The thesis project will focus on the synthesis and characterization of novel carbon-based materials for energy conversion applications, including nuclear energy. The student will explore different synthetic approaches and get training in specialized characterization techniques.

Prof. Olena Zenkina

1. Preparation of surface confined materials for selective metal ion sensing and removal of heavy metals/





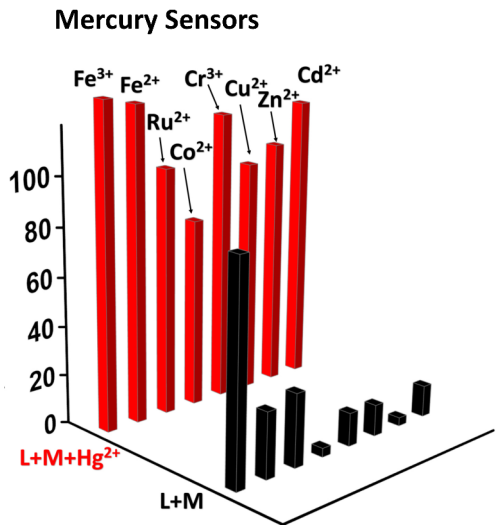


Figure 1: Metal ion sensors on metal-oxide nanosurfaces. A: Fe^{2+}; B: $Hg^{+/2+}$, Pb^{2+}, $As^{3+/5+}$. C: Removal of metal ions.

Laschuk N. O., Ebralidze I. I., Quaranta S., Kerr S., Egan J. G., Gillis S., Gaspari F., Latini A., **Zenkina O.V.**, *Materials & Design*, **2016**, *107*, 18–25.

Laschuk N. O., Ebralidze I. I., Spasyuk D., Zenkina O. V. "*Eur. J. Inorg. Chem.* 2016, *22*, 3530-3535.

Undergraduate student authors marked in red

Prof. Olena Zenkina and Prof. Brad Easton

2. The preparation of coordination based functional electrochromic materials and metal wires on the conductive surfaces.

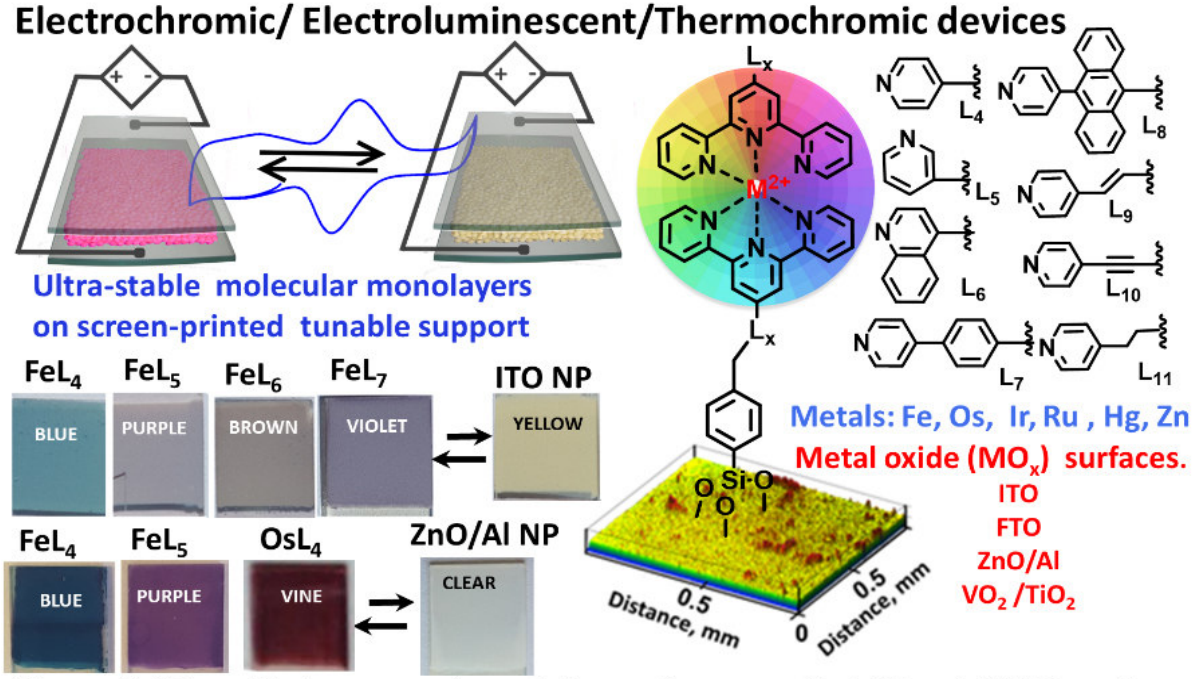


Figure 3. "Smart" chromogenic metal complexes on "intelligent" MO_x surfaces.

Laschuk N.O., Ebralidze I.I., Poisson J., Egan J.G., Quaranta S., Cusden H., Allan J.T.S., Naumkin F., Gaspari F., Easton B., Zenkina O.V. *ACS Applied Materials & Interfaces.* **2018**, *10* (41), 35334–35343

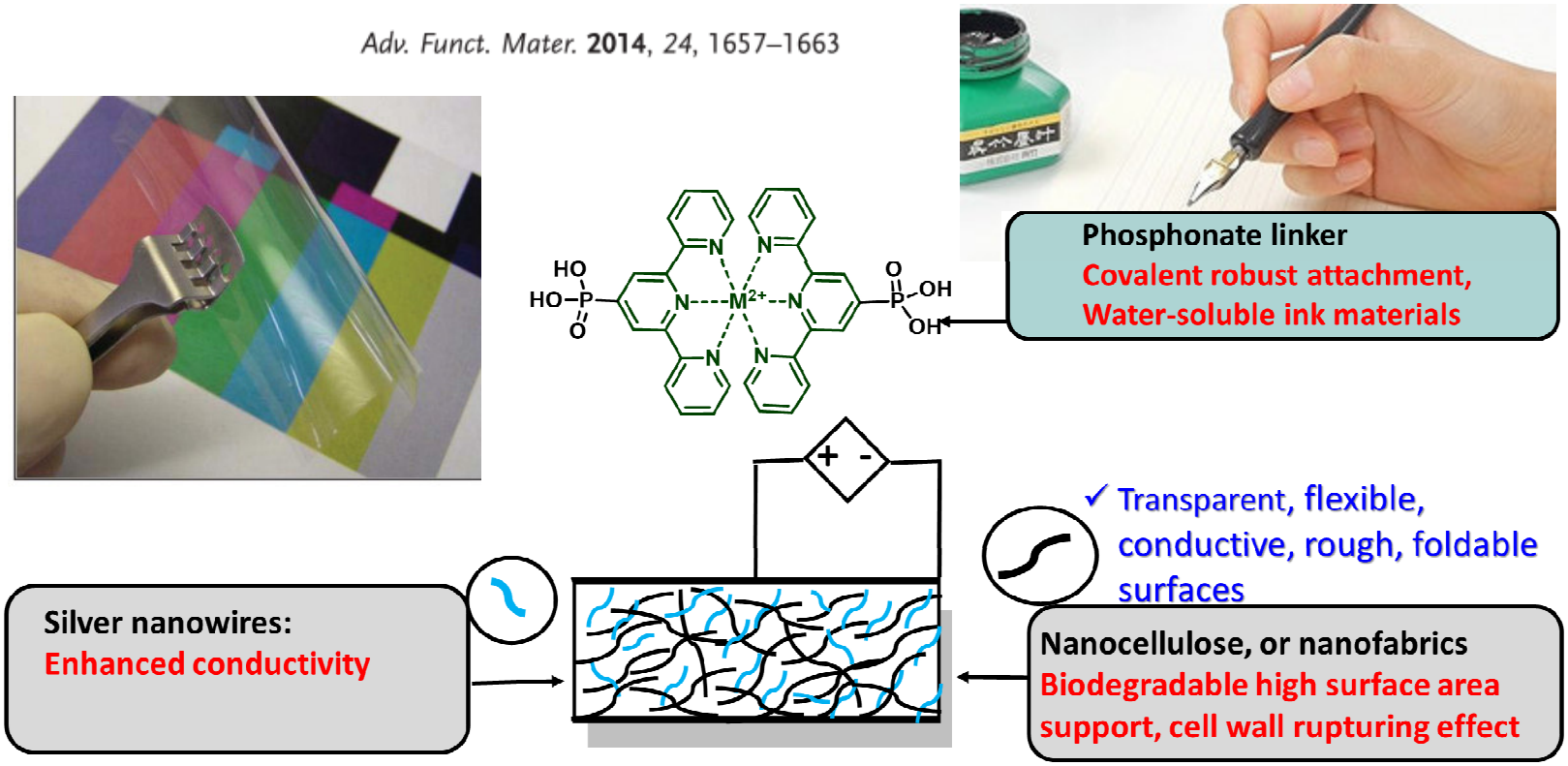
Poisson, J.; Geoffrey, H. L.; Ebralidze, I. I.; Laschuk, N. O.; Allan, J. T. S.; Deckert, A.; Easton, E. B.; Zenkina, O. V., *J. Phys. Chem. C* **2018,** (122), 3419–3427.

Allan, J. T. S.; Quaranta, S.; Ebralidze, I. I.; Egan, J. G.; Poisson, J.; Laschuk, N. O.; Gaspari, F.; Easton, E. B.; Zenkina, O. V., *ACS Applied Materials & Interfaces* **2017,** *9* (46), 40438-40445.

Undergraduate student authors marked in red

Prof. Olena Zenkina

3. Nanocellulose based conductive surfaces for smart molecular materials.



We interested to make a water-soluble ink of different colours from well-defined transition metal complexes and to be able to "write" (covalently introduce electrochromic molecules) on the transparent biodegradable nanopaper. Novel materials may allow an easy electrochemically switching between colours and/or erasing of colours.

We target erasable, bendable transparent, multicolour electrochromic paper.

This is totally new research direction in our group.

We will closely collaborate with group of Prof. Easton on Electrochemistry side of this project!