4th-year Thesis Projects in Chemistry
University of Ontario Institute of Technology
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Professor Yuri Bolshan, Assistant Professor – Research Profile

The Bolshan’s organic/pharmaceutical chemistry research group aims at the development of novel reactions and their applications to the synthesis of pharmaceutically relevant molecules.

**Project 1:** We are interested in the functionalization of benzhydryl moieties since this scaffold is present in numerous pharmaceuticals. Our newly developed methodologies allows for a facile derivatization of benzhydryl moiety with high functional group tolerance.

![Chemical Reaction](image)

**Project 2:** In addition, we are working on direct functionalization of sugars, which is a challenge for today’s medicinal chemists. Forming a carbon-carbon bond at the anomeric position significantly improves chemical and enzymatic stability. Thus far, we achieved direct functionalization of unsubstituted furans.

![Chemical Reaction](image)

**Selected Publications Involving Undergraduate Students**


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.

**Project 1. Chemical Synthesis of Novel Short-Interfering RNAs**

In this project, an undergraduate thesis student will work closely with other members of the lab, aimed at synthesizing new types of chemically-modified short-interfering RNAs. 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 thesis student to wide range of experimental techniques in a state-of-the-art laboratory. Note, other undergraduate projects also available in chemical biology in Dr. Desaulniers’ lab.

**Selected Publications Involving Undergraduate Students (bolded)**

1) J.-P. Desaulniers, G. Hagen, **J. Anderson**, C. McKim, **B. Roberts**. "Effective Gene-Silencing of siRNAs that Contain Functionalized Spacer Linkages Within the Central Region" *RSC Advances 2017*, 7, 3450-3454.


**More information**: Visit [http://faculty.uoit.ca/desaulniers/home.htm](http://faculty.uoit.ca/desaulniers/home.htm).
The Easton research group is focused on the development of new materials & methods for electrochemical systems, with specific application in energy & sensory devices. In particular, we seek to develop new materials with specific properties that can either address or provide insight into the scientific challenges faced by these technologies. Carbon is ubiquitous with high surface area porous electrodes, finding applications as a catalyst support in fuel cells, & also forming the primary component in many supercapacitors. Typically these nano-sized carbon particles (10-50 nm) form porous 3-D structures, often held together with a polymer binder. Several projects in the Easton lab focus on specific covalent surface modification reactions that can have a substantial impact on both the electrochemical performance and stability of these materials. This, along with the development of in situ electrochemical diagnostic techniques enable real time assessment of the extent of modification and/or the extent of degradation. This work will enhance the fundamental understanding of electrode structures for energy conversion & storage devices and also advance the design of electrodes with improved performance and durability.

Project 1. Carbon electrode degradation in the presence of anion contaminants
Working closely with other lab members, the undergraduate thesis student will study carbon electrode stability in the presence of anion contaminants such as Cl\(^-\) and F\(^-\). In particular, the rate of degradation will be examined under conditions (temperature, pH, etc.) that mimic real world operating conditions for fuel cells, & electrolyzers, supercapacitors. Furthermore, the student will examine the influence the anion has on the stability of specific surface moieties, and also monitor changes to the electrode structure through ex situ characterization (e.g. XPS, Raman, FTIR, XRD, etc.). This project will expose the undergraduate thesis student to a broad range of techniques in materials chemistry in a state-of-the art electrochemistry research lab.

Selected Publications Involving Undergraduate Students

Professor Fedor Naumkin, Associate Professor – Research Profile

The Naumkin’s Computational Nanochemistry research group deals with prediction and design of new nanosystems (atomic and molecular complexes and clusters), analysis of their structures, properties, and their inter-relationships. Of specific current interest are novel systems with molecules trapped (1) between counter-ions or (2) inside metal cluster cages, with parameters of both these “core” and “shell” components evolving. Such species could have various applications including new tuneable nanocatalysts, building blocks with desired shapes and electronic properties, sensitive light detectors, molecular electronics and machinery, efficient matter and energy storage at molecular level, new materials, molecular self-assembly, new type of induced reactions, etc.

Project 1. Modelling of systems of ion-pair-trapped molecules for added polarity and assisted molecular assembly.

The student will computationally investigate a series of insertion complexes of molecules in ion-pairs. These systems are to be suitably designed based on the inserted-molecule geometries, their structures optimized in terms of energy, and stability and other properties analysed. Next, a few such units will be assembled into a larger aggregate. In each case, the system behaviour in ionic and electronically-excited states will be studied as well, to evaluate feasibility of charge/excitation–controlled manipulation. The obtained results will be used to predict further modifications of the system structure and composition in order to achieve anticipated outcomes or enhance discovered ones. The student will acquire practical experience of working with the state-of-the-art quantum-chemistry software and modern visualization tools, on high-performance computing facilities accessible at the UOIT and Sharcnet network of Ontario.

Selected publications with undergraduate students


3) P. McNelles* and F. Y. Naumkin, A small molecule in metal cluster cages: H$_2$@Mg$_n$ (n=8-10). Phys. Chem. Chem. Phys. 11 (2009) 2858-2861

More information: Visit http://myweb.science.uoit.ca/~fnaumkin
Professor Liliana Trevani - Associate Professor - Research Profile

The Trevani research group on advanced materials for energy generation and conversion uses tools of several branches of chemistry to address relevant scientific challenges in the fields of hydrogen production, energy conversion devices, and high-temperature electrochemistry; in many cases in collaboration with other groups due to the interdisciplinary nature of the projects. The group specializes in the design, development, and application of home-built state-of-the-art spectroscopic and electrochemical methods for the synthesis and characterization of materials under high temperature and pressure conditions to offer new venues for the study of materials and industrial chemical processes.

Project 1: Synthesis and characterization of nanocatalysts and proton conducting membranes for high-temperature fuel cells.

The student’s project will be oriented to the synthesis of catalyst and membrane composites for high-temperature polymer electrolyte membrane fuel cells. The student will get hands-on experience in materials chemistry while learning sophisticated characterization techniques, from classical electrochemical methods such as cyclic voltammetry and impedance to spectroscopic techniques. Also, the project will bring the student the opportunity for getting training on experimental design and critical data analysis. Depending on the results the student will present his/her findings at the South Ontario Undergraduate Chemistry Conference.

Selected Publications


More information: visit http://www.liliana-trevani.com/
The Zenkina research group in Materials Chemistry focuses on the development of novel nanostructures employing self-assembly of organic and organometallic compounds on metal and oxide surfaces with a heavy emphasis on their practical applications as metal ion sensors, protein receptors, and electrochromic materials. Our research efforts are focused on the development of assays that allow simultaneous multi-analyte detection. To reach this goal, we introduce various nitrogen-containing building blocks into one multidentate molecule able to simultaneously detect few drastically different metals. On the other hand, we built ligands able to interact with metal centers of metalloproteins producing a Uv-vis and/or fluorescence readouts that can be analyzed and interpreted using logic gates concept.

**Project 1. Preparation of surface confined materials for selective metal ion sensing.**

In this project, an undergraduate student will work closely with other lab members, on the synthesis of novel ligands and their deposition on surfaces. We will determine binding affinities and establish stoichiometry of the ligands coordination to a variety of metal ions. Self-assembled monolayers formed from these novel ligands will be further interacted with aqueous solutions of suitable metalloproteins. Students who advance this research will learn organic, inorganic, analytical, physical, and surface chemistry; will get strong experience in applying their knowledge to design new materials starting from synthesis of molecular building blocks, assembly them using various binding motifs, and analyze the optical response of the developed sensor interacting with variety of analytes.

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

For this project an undergraduate student will prepare variety organometallic self-assembling multilayers on semiconductor surfaces (indium tin oxide nanoparticles, ITO/glass). Subsequently, he or she will fine-tune the colour of our assemblies by rational ligand modification. Changing the nature of the organic functionalities by introducing a conjugated organic moiety, quaternization of the outer pyridine ring, or changing the metal will significantly affect metal to ligand charge transfer and as a result change the colour of the metal complex. Bottom-up layer-by-layer deposition will be used to grow homo- and heterometallic molecular wires (M: Fe, Os, Rh, Ir) with tunable colour and charge transfer properties. The student will explore
chemical and electrochemical switching properties, stability, conductivity and colour efficiency of these novel materials. *The ultimate goal will be to create functional materials with high coloration efficiency, colour homogeneity, high contrast ratios and controllable switching time.* Electrochemical measurements will be conducted in collaboration with Prof. Brad Easton.

Students who advance this research will learn inorganic and organic synthesis, methods for materials preparation and characterization and main strategies for studying and optimization of metal-ligand interactions on the surface support.

**Project 3: Controlled immobilization of plasmonic metal nanoparticles (NPs) on the flat and porous semiconductor surfaces.**

Plasmonic gold or platinum nanoparticles stabilized by weakly coordinating ligands (water soluble citrate-capped NPs, etc.) will serve as metal nanosurfaces. Simple bifunctional organic linker 1 will be used to bring together semiconductor and metal surfaces that will allow to comprise both the optical properties of plasmonic metal NPs and the wide band gap properties of semiconductors (ITO/TiO$_2$). Siloxane moiety will form stable assemblies on hydrophilic surfaces while N-heterocyclic carbene group has high affinity to various metals. Novel structures will be examined for their catalytic applications (reduction of nitro-aromatic compounds etc.), as chemo- or biosensors and/or materials for molecular electronics. Students who advance this research will learn inorganic and organic synthesis, methods for nanoparticles preparation and characterization and main strategies for studying and optimization of catalytic transformations on nanoscale surfaces.

**Selected publications.** (Undergraduate student authors marked in red).


**More information:** Visit [http://faculty.uoit.ca/zenkina/](http://faculty.uoit.ca/zenkina/)
Work in the MJA Lab is focused on synthetic organic chemistry with projects ranging from the biologically applied to synthetic methods development to fundamental physical organic chemistry. In general we are interested in connecting molecular structure to function, and using our knowledge of each to push the boundaries of the other no matter what the application. Research in The MJA Lab is currently being performed at Northern Illinois University (DeKalb, IL, USA).

Project 1: Silatrane as a practical and useful atom-transfer reagent

Silatranes are fascinating structures that contain a stable pseudo-pentavalent silane. Many aspects of silatrane chemistry have been well-studied, though one relative gap of information exists with regard to their reactivity as atom-transfer reagents – an application which is common to many other silanes. The MJA lab has recently began to explore reactions involving the transfer of hydride (i.e. reduction), and would like to both understand this process better and apply the principles of silatrane reactivity that we have learned to enable to reaction of other types of groups. A thesis student interested in this project would be able to select from a variety of possible endeavors related to this central theme.

Selected Publications Involving Undergraduate Students

Guidelines for Selecting a Thesis Supervisor

If you are interested in a chemistry honors thesis, setup an appointment with a prospective supervisor to discuss the possibility of working in their laboratory as a thesis student. You can make up to three different choices. The first two choices must be from a Tenured or Tenure-Track Faculty member (TTTF). The third choice can be from either a TTTF or a Teaching Faculty (TF) member. Below are the TTTF members and TF members supervising chemistry thesis projects for 2017-2018.

**TTTF:**
Dr. Bolshan  
Dr. Desaulniers  
Dr. Easton  
Dr. Naumkin  
Dr. Trevani  
Dr. Zenkina  

**TF:**  
Dr. Adler  

Hand in the thesis application form to Dr. Desaulniers, or Tara Funston (Student Advising) before April 30, 2017. Dr. Desaulniers will inform you of the decision sometime in May.