Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

2018 iSURE PROJECTS

In the online application, please select **up to 3** research projects in Question 39 (press Ctrl while selecting). Then, rank them in order of priority in the text box of Question 40 before your essay.

Department of Physics

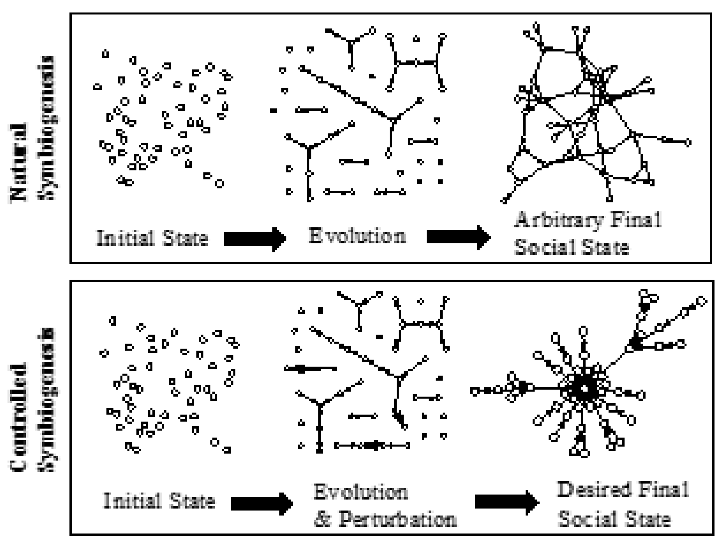
1. Ecological Control Theory

Evolutionary control has a long history starting with agricultural domestication and culminating into contemporary genome editing technologies. However, this history is largely limited to controlling individual species. We view ecological and biosocial networks as the new circuit board, and evolution as a manufacturing process capable of fabricating *eco-machines.* Evolutionary control promises terraforming worlds, degrading pollution, and manufacturing astonishing compounds.

This is a theoretical / computational project that aims to establish an analytical framework to steer the evolution of multiple populations that strongly interact with one another. Specifically, we wish to theoretically understand how to manipulate the connectivity of networks representing ecological or biosocial webs, which range from bacterial biofilms to rainforests. The project particularly focuses on ecological control under noisy or incomplete knowledge of the existing interactions and population levels of species.

The project requires mathematical and computational dexterity. Applicants are expected to be familiar with matlab, differential equations/ dynamic systems, and elementary probability theory.

Figure 1. Schematics of Evolutionary Control. Our goal is to develop a theory that will allow manipulating biosocial evolution by topological and parametric perturbations. The fundamental object we aim to control is not populations, but the structure of interactions.



Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

Department of Chemistry and Biochemistry

2. **Late-Transition Metal Pincer-Type Complexes Involving Metal-Ligand Cooperation for Alkane and Small Molecule Activation**

Catalysis is at the center of green chemistry efforts, especially when it involves readily available feedstock such as water, alcohols, and amines. An approach with major practical implications is the selective functionalization of E-H (E = O, N, C, Si, B) bonds since syntheses can be simplified and less waste generated than with traditional methods. Oxidative addition of such bonds will be investigated. Our new approach involves metal-ligand cooperation, specifically, hydrogen transfer from the ligand to the metal and vice versa, which allows transformations under mild conditions.

3. **Synthesis of Hyperbranched Polymers with Well-Defined Nanostructure**

Highly branched polymers, e.g., hyperbranched polymers, are a class of popular soft nanomaterials that have attracted broad interest due to their easy synthesis, three-dimensional structures and multiple periphery groups. They have demonstrated promising properties for a variety of applications in catalysts, sensors, hybrid nanoparticles and drug delivery. However, the structure of hyperbranched polymers in traditional one-pot synthesis was often poorly defined, which affects their physical properties and limits their advanced applications. Our group recently developed a method for synthesis of hyperbranched polymers with high molecular weight, narrow molecular weight distribution and high degree of branching in a one-pot chain-growth polymerization. The iSURE student is expected to get involved in this project to screen different monomers to understand the polymerization mechanism and explore new types of polymerization conditions to achieve similar and even better control of the polymer structures

Department of Biological Sciences

4. **The Evasion of Detachment-Induced Metabolic Defects in Breast Cancer**

Metastasis, the spread of cancer from the site of the primary tumor to distant locations in the body, is responsible for 90% of cancer deaths, yet the molecular mechanisms governing this extraordinarily complicated process remain poorly understood. It has become clear that an important barrier to metastasis is the induction of anoikis, a cell death process that is induced when epithelial cells lose attachment to the extracellular matrix (ECM). During the course of tumor progression, cancer cells will typically acquire resistance to anoikis which can facilitate the spread of these cells to distant sites. In addition to the induction of the anoikis program, we have discovered that ECM-detached cells are metabolically compromised in a fashion that prohibits their survival. Thus, ECM-detached cancer cells need to inhibit anoikis and rectify their metabolic deficiencies in order to survive. Despite its importance, there is a striking lack of information on how cancer cells successfully evade the induction of anoikis and overcome metabolic deficiencies. The overarching goal of our lab is to examine and characterize the biological mechanisms that permit cancer cell survival in the absence of ECM attachment. It is our hope that a better understanding of these mechanisms at the molecular level will reveal novel chemotherapeutic targets or approaches that may serve to compromise the survival of ECM-detached cancer cells and thus prevent tumors from successfully metastasizing.

Department of Computer Science and Engineering

5. From Big Data to Small Data: Taming the two V's of Veracity and Variety

Data of questionable quality has led to significantly negative economic and social impacts on organizations, leading to overrun in costs, lost revenue, and decreased efficiencies. The issues on data reliability, credibility, and provenance has become even more daunting when dealing with the variety of data, especially data that are not directly collected by an organization, but from the third-party sources such as social media, data brokers, and crowdsourcing. To address such issues, this project aims to develop a Data Valuation Engine (DVE) that solves the critical problem of data reliability, credibility and provenance, and provides accountability and quality processes right from data acquisition. The DVE leverages and innovates techniques in estimation theory, data fusion and machine learning to fill a critical gap in data accountability and quality, thereby providing a transformative step in countering the ubiquitous data quality issues found in almost every application domain from business to environment to health to national security. The DVE will be integrated in the Hadoop ecosystem and will be agnostic to the data source, application or analytics, and provided as a hosted solution to the community.

6. Visual Data Analytics

Need iSURE students familiar with programming in C/C++, OpenGL/GLSL/WebGL, or D3.js will assist in the design and implementation of visualization and analytics programs for analyzing and understanding a wide variety of data (e.g., simulation data, social media data), and for teaching and learning essential visualization concepts and techniques.

Department of Electrical Engineering

7. Design and Analysis of High-Performance Compound Semiconductor Devices

Numerical simulation and optimization of high-performance III-V compound semiconductor devices will be performed. Specific devices include photovoltaics, high-speed transistors, high voltage diodes and transistors, and novel devices for low-power digital and signal processing.

8. Fabrication Process Development for High-Performance Devices

Student will contribute to development of fabrication processes for high-performance III-V compound semiconductor devices, working in Notre Dame's cleanroom facility. Specific devices include high voltage diodes and transistors, as well as RF/microwave devices.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

9. Energy Recovery for Ultra-Low Energy Computation

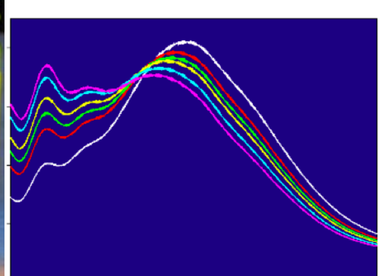
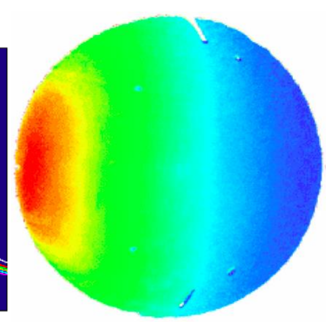
Anyone who owns a laptop knows that power dissipation and the associated heat are a problem for the microelectronics industry. As electronic devices scale down in size, they use less power (and hence energy), but is there a lower limit to the energy that must be dissipated by each device? Recent experimental measurements have demonstrated our ability to measure energy dissipation in the range of a ~15 yJ (1 yJ is 10-24 J), and we are building CMOS circuits to operate in this range. Projects in this group will explore the limits of ultra-low power computing, and designing, building and measuring circuits that test these limits, and clock circuits that can recycle the energy used in computation. The projects will include building circuits and amplifiers for energy measurements of the CMOS circuits as well as the actual measurements. The project will also include the design of the next generation of the adiabatic circuits. A student involved in these projects will gain experience in programming, CMOS design, and device measurement techniques. Students will work on the construction of circuits, writing control programs, and making measurements. Students in electrical engineering, physics, and computer science students are preferred. Some knowledge of programming and soldering is helpful.

Department of Aerospace and Mechanical Engineering

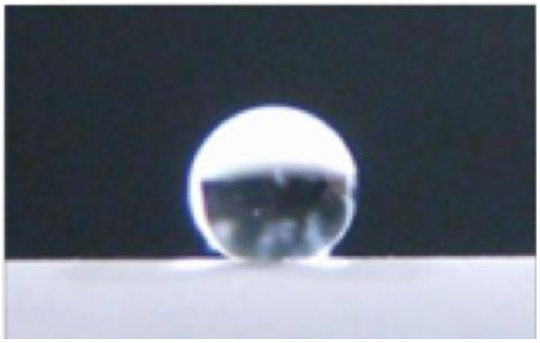
10. Functional Chemical Sensor and Coating for Fluid Dynamic Applications

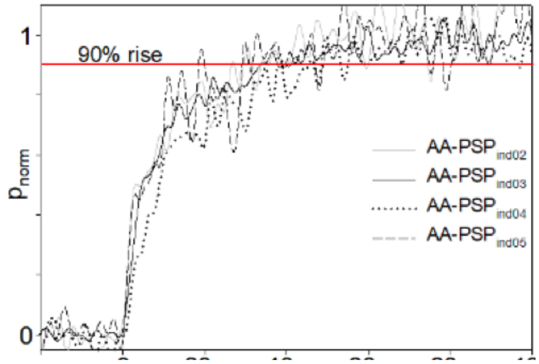
This project is an interdisciplinary topic on chemistry and fluid dynamics. The spectrum of this project has three steps: development, characterization, and application. Depending on a topic involved, a research focus for an applicant will be varied within these three steps.

A luminescent chemical sensor and hydrophobic coating are focused on the development step. In characterization step, sensor and coating performances will be related to fluid dynamic quantities, such as static and dynamic changes in pressure and temperature. Application step will be performed using a shock tube.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.





The expected and/or anticipated involvement of research interns: A student will be involved in a chemical sensor and/or coating development, the characterizations of the developed sensor/coating using spectrometer and pressure/ temperature-controlled device. The developed sensor will be tested in a shock tube.

Preferred discipline, expertise, lab skills from research interns: A student from the following discipline is preferred: chemistry, chemical engineering, industrial engineering, mechanical engineering, and aerospace engineering.

11. Fabrication of Polymer Nanofibers with Anomalous Thermal Conductivity

Amorphous polymers are known as thermal insulators with a thermal conductivity of ~0.1-0.3 W/mK. However, they can be more thermally conductive than many metals if we can reform them into highly aligned nanofibers (thermal conductivity > 50 W/mK). This suggests that polymers can be used to replace metals in many heat transfer devices and equipment, such as in electronic packaging and heat exchangers, with the additional advantages of reduced weight, chemical resistance, and lower cost. In this project, undergraduate researchers will fabricate polymer fibers with nanometer diameters by ultra-drawing fibers from polymer melt. They will also characterize the nanofibers using electron microscopes and X-ray scattering, and measure thermal transport properties using scanning thermal microscopy.

Department of Psychology

12. Statistical Social Network Analysis for Behavioral Research

Network analysis is becoming a popular interdisciplinary research topic in computer science, statistics, sociology, political science and psychology. In our lab, we study the covariates that are related to the formation and development of networks, such as a friendship network, as well as how a network is related to behavioral outcomes such as smoking and alcohol use. We develop new models and software using both Bayesian and frequentist's methods for better network data analysis.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

13. Cognitive Neuroscience of Memory & Aging Lab

We have several ongoing projects examining memory and aging using behavioral testing, neuroimaging (EEG/ERP, fMRI), neurostimulation (TMS, tDCS), and Virtual Reality methods, as well as statistical modeling (MVPA, CFA, SEM), to develop and test theories of memory. Our research is generally focused on memory and age-related changes in memory. In particular, we study the behavioral and neural processes associated with working memory and the relations among working memory, episodic memory, prospective memory, and higher-order cognition (e.g., fluid intelligence, language comprehension). We study these topics in various populations including young adults, healthy older adults, and in patients with Alzheimer's Disease, Parkinson's Disease, amnesia, or concussion/traumatic brain injury. In addition to studying basic memory processes, our research also assesses how cognitive theories can be applied to understanding memory performance in the real world and how cognitive training techniques can be utilized to improve memory performance.

In your application, please comment on proficiency with computer programming. Experience with Matlab, Python, and/or Unity is highly desired. Responsibilities will include helping lab members prepare applications, program experiments, run experiments / collect data, process data, and attending lab meetings.

14. Polymer Electrolytes for Advanced Rechargeable Batteries

The objective of the research is to investigate solid polymer and/or polymer gel electrolytes for use in lithium and/or magnesium rechargeable batteries. Such electrolytes have to potential for increase battery safety due to their lower volatility and higher thermal stability compared with commercial electrolytes. Current polymer electrolytes suffer from low ionic conductivities that result in low battery charge/discharge rates, which preclude their use in commercial devices. The REU student will prepare materials and characterize the electrochemical, transport, mechanical, and/or and thermal properties of these new materials. Prior lab experience and a background in chemical engineering, chemistry, materials science, or a closely related field is preferred.

15. Special Project: For directly nominated students only. Please do not select this project unless told to do so.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

2018 iSURE PROJECTS
Within the Center for Nano Science and Technology

Department of Physics

16. Sub cellular particle analysis with Light Transmission Spectroscopy

This research will employ a new technique, Light Transmission Spectroscopy, to determine the size distribution of sub-cellular particles in the range of ~ 2 to 3000 nm in diameter. This includes objects ranging from proteins to organelles. The object is to gain a new insight into cellular functioning and inherent topology based on the particle distribution within both plant and animal cells. One existing application has been in determining differences in cancer versus normal cells. The student will help prepare and measure cell lysates (contents), prepare samples by centrifugation and filtering, analyze data, etc. Some basic bio. lab., computer, and general data analysis skills helpful.

Department of Chemical and Biomolecular Engineering

17. Engineering multifunctional nanoparticles for targeted drug delivery in cancer

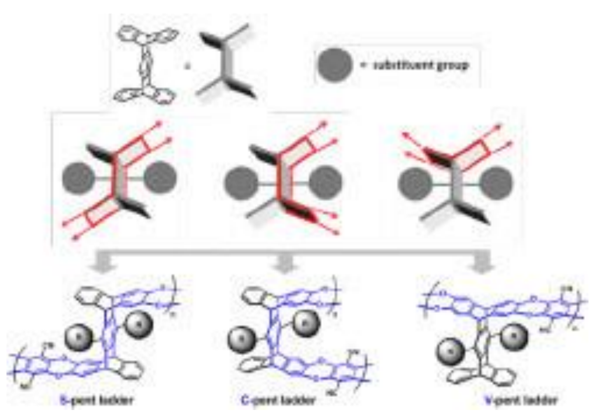
Modern cancer therapeutics are typically developed to aim at key pathways and proteins that are critical to the survival and progression of malignant cells. Nevertheless, they are still associated with undesirable side effects due to non-specific toxicity that non-targeted tissue and organs experience. In recent years, nanoparticle (NP) based drug delivery systems that carry drugs to tumors in the body have greatly improved the efficacy of traditional therapeutics while decreasing the associated systemic toxicities. NPs with a diameter of 10-200 nm can selectively target and preferentially home at the tumor site via the enhanced permeability and retention (EPR) effect. More complex NPs, such as multiple drug carriers (for combination therapy) and coatings of targeting elements for receptors on cancer cells, have also been engineered to improve the overall outcome by overcoming problems associated with tumor tissue targeting and penetration, drug resistance, cellular uptake and circulation half-life. We use NPs to target multiple myeloma (MM), a B-cell malignancy characterized by proliferation of monoclonal plasma cells in the bone marrow (BM) and is the second most common type of blood cancer in the U.S. Despite the recent advances in treatment strategies and the emergence of novel therapies, it still remains incurable. A major factor that contributes to development of drug resistance in MM is the interaction of MM cancer cells with the BM microenvironment. It has been demonstrated that the adhesion of MM cells to the BM stroma via $\alpha 4\beta 1$ integrins leads to cell adhesion mediated drug resistance (CAM-DR), which enables MM cells to gain resistance to drugs such as doxorubicin (Dox)–a 1st line chemotherapeutic in the treatment of MM. To overcome this problem, the clinicians apply combination therapy, which is the simultaneous use of two complementary chemotherapeutic agents during treatment. One caveat of this treatment method has been that it is almost impossible to attain the critical stoichiometry at the tumor that is necessary to achieve this synergistic drug effect when conventional methods of chemotherapy are used. Here, we seek to overcome this challenge by using an engineering approach for targeted drug delivery. The overall objective of this proposed project is to engineer "smart"

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

nanoparticles that will deliver and exert the cytotoxic effects of the chemotherapeutic agents on MM cells, and at the same time do it in such a manner as to overcome CAM-DR for improved patient outcome. To enable this, we will engineer micellar nanoparticles that will be (i) functionalized with α4β1-antagonist peptides as well as Dox and carfilzomib drug conjugates, and (ii) designed to show the adhesion inhibitory and the cytotoxic effects in a temporal sequence. When the nanoparticles are delivered to the MM cells, as a first step they will interact with the cell surface α4β1 integrins and inhibit MM cell adhesion to the stroma, thereby preventing development of CAM-DR (Fig. 1). In the second step, the chemotherapeutic agents will exert their synergistic cytotoxic effects after cellular uptake, as the nanoparticles will be designed to require a low pH environment such as the endocytic vesicles, to release active drugs. This way, the "smart" nanoparticles will act on the MM cells in a temporal fashion and prevent development of CAM-DR for improved patient outcome.

18. Polymer membranes with tunable microporosity for gas separations

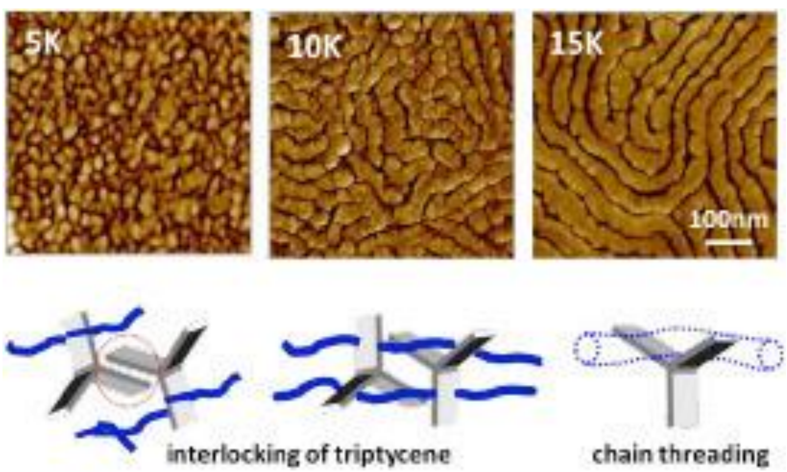
Polymers with well-defined microporosity are highly desired for gas separation membranes, wherein high microporosity enables fast gas transport while the finely tuned pore size regulates selective transport via size sieving. Recently there have been markedly increasing research interests in developing microporous polymers for gas separation membranes, such as polymers with intrinsic microporosity (PIMs). However, the reportedly super high gas permeability of microporous polymers always accompanies with low selectivity, mainly due to the lack of precise control over pore size distribution in these polymers. Moreover, physical aging induced deterioration of permeability remains as one of the biggest challenges for microporous polymer membranes. This project will focus on constructing highly rigid ladder-like polymers using a shape-persistent building block based on pentiptycene-containing structural units. The novelty of this new type of microporous polymers lies in the truly intrinsic microporosity defined configurationally by the shape of the pentiptycene units, which offers unique opportunity to tailor the microcavity architecture in the membranes and simultaneously provide superior resistance towards physical aging by taking advantage of the rigid framework of pentiptycene moieties. The project will involve the synthesis of pentiptycene-based monomers with various bridgehead substituent groups, polymerization of tetra-functional pentiptycene monomers with commercial comonomers, membrane fabrication/characterization, and pure-gas permeation tests. A student in materials science, chemical engineering, or chemistry is preferred, and having previous experience in a chemical laboratory would be helpful.



Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

19. Nanostructured polysulfone polyelectrolyte copolymer membranes for fuel cells

Sulfonated polysulfone copolymers with controlled nanophase-separated morphology hold great potential as alternatives to benchmark Nafion® for polyelectrolyte membrane fuel cells (PEMFCs), due to their much better proton conductivity at low relative humidity (RH) levels and thermal stability. Previous research has shown that long hydrophilic (ionic) sequences or high degree of sulfonation are needed to form well-connected proton conducting nanochannels that enables high proton conductivity at low RH. However, it invariably comes at the expense of high water uptake and excessive membrane swelling resulting in deterioration of the dimensional stability and mechanical robustness. This project aims to exploit an innovative supramolecular strategy to address this water management challenge in PEM membranes via introducing triptycene-based building blocks into polymer backbones. It is expected that supramolecular interactions of chain threading and interlocking induced by triptycene units can effectively suppress water swelling while maintaining high water uptake, which is critical to provide high proton conductivity under low RH conditions. Specifically, both random and multiblock copolymers of systematically varied compositions will be developed in this project to investigate how supramolecular interactions of triptycene units govern the formation of proton-conducting nanochannels as well as proton transport properties. The project will start with the synthesis of triptycene diol monomer, which will be copolymerized with commercial sulfonated monomer to produce both random and multiblock copolymers. Comprehensive characterizations of the copolymers will be conducted to confirm the chemical structure (NMR and FTIR) and access their thermal and mechanical properties (DSC, TGA, tensile test, etc.). Membrane fabrication and acidification will then follow to prepare free standing, defect-free films for water swelling measurement, morphology characterization (AFM, TEM) and proton conductivity measurements (impedance spectroscopy). A student in materials science, chemical engineering, or chemistry is preferred, and having previous experience in a chemical laboratory would be helpful.



Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

20. Fabrication of solid state batteries

Solid state batteries (SSBs) may be a key enabler for electric vehicles. A solid electrolyte can overcome many shortcomings of present technology including offering wider electrochemical voltage ranges, better chemical compatibility, and improved safety. Progress is needed to overcome electrolyte limitations and provide more economical processing while still delivering sufficient energy density for automotive applications. ND researchers are developing ceramic electrolyte materials (Li7La3Zr2O12) and low-cost processing methods to provide for high-power, solid-state, lithium-ion batteries for use in EVs. A key factor to drive down costs is the development of scalable, ceramic fabrication techniques. The goal of this project is the fabrication of thin Li7La3Zr2O12 electrolyte sheets through the synthesis, tape casting and sintering of nanosized electrolyte and electrode powders. These electrolyte sheets are then assembled into cells for subsequent development of rapid charging solid state batteries.

The student will synthesize (chemical processing) and characterize (X-ray diffraction, dilatometry) nano-sized powders of battery component materials (electrolytes, electrodes). Slurries for tape casting will be prepared and sintered. Cast tapes will be characterized (impedance spectroscopy). Batteries will be fabricated from tapes (glove box work). Students in materials science, chemical engineering, or chemistry preferred.

21. Construction and demonstration of an atomic layer deposition system for synthesis of supported nanoparticle catalysts

Atomic layer deposition (ALD) is a promising technique for catalyst synthesis because it allows for atomic-level control over the structure and composition of the catalyst. While ALD systems are commercially available, they are expensive (>$100k) and cannot be easily modified for custom research applications. Alternatively, ALD systems can be built in the laboratory at much lower cost and with much greater flexibility than the commercial systems. The objectives of this project are (1) to build a custom-made reaction system that couples ALD synthesis of catalytic materials with in-situ spectroscopic characterization of the catalyst structure, and (2) to demonstrate the basic capabilities of the system by depositing thin metal-oxide (e.g., Al2O3) films onto planar substrates. The student will be involved with the construction of the ALD system from its constituent parts (valves, tubes, heating elements, controllers, etc.) and also the controlled deposition of thin metal-oxide films using the ALD system. Laboratory experience, particularly in building or modifying scientific equipment, is preferred though not required.

22. Elucidating fundamental processing-property relationships for chemically patterned membranes generated using inkjet printing technologies

Membranes based on self-assembled block copolymer precursors are an emerging class of promising separation and purification devices, which will find application in water treatment, pharmaceutical purification, and biofuel processing applications, due to the ability of researchers to control the nanostructure and chemistry of these multifunctional materials. To date, the most successful methodology for directing the assembly of nanostructured copolymer-based

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

membranes has been the self-assembly and nonsolvent induced phase separation (SNIPS) procedure. In addition to being facile and scalable to industrial-scale manufacturing processes, the versatility of the SNIPS process makes it an attractive membrane fabrication methodology. In particular, the membrane nanostructure and chemistry generated by the SNIPS process can be tuned in a ready manner by simply varying a number of engineering parameters. Recently, it was demonstrated that this flexibility could be exploited to chemically pattern the surface of copolymer membranes using inkjet printing devices, which resulted in the emergence of novel transport properties. As this nascent field develops, it is critical to develop fundamental knowledge regarding how the copolymer membrane nanostructure and the inkjet printing protocols correlate with the properties that emerge from the patterned membranes. As such, the objective of this project is to identify the key material relationships that control the interplay between membrane nanostructure, functionality, and transport properties of chemically patterned membranes. This knowledge will allow us to refine the printing process for the optimization of membranes with targeted performance profiles. The student researcher will be asked to fabricate membranes using the SNIPS process, modify the surface chemistry using inkjet printing devices, and elucidate how the nanoscale structure and chemistry of the membranes impact the observed transport properties through experimental water flow and solute throughput tests. Chemical, Mechanical, Electrical, and Environmental Engineers are well-suited to undertake this research project.

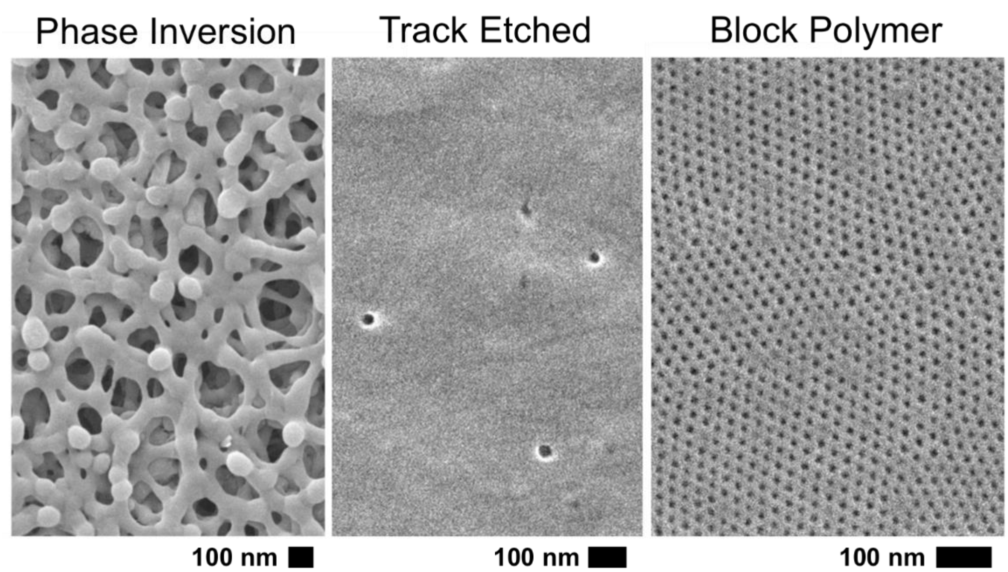


Figure 1: Typical structures of three size-selective membranes.

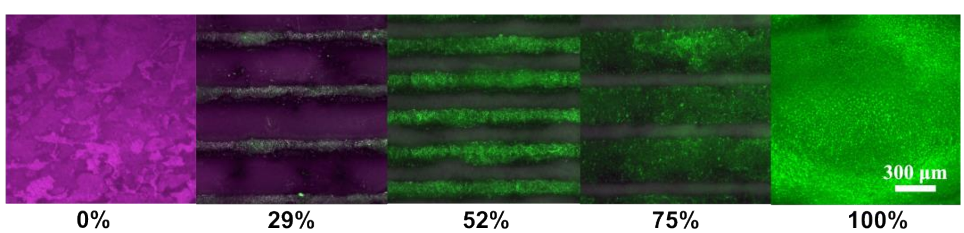


Figure 2: Micrographs of chemically-patterned copolymer membranes.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

23. Targeting therapeutics through supramolecular affinity

We are motivated to advance the practice of therapeutic nanotechnology by capturing several of the benefits of antibody targeting while avoiding some known complications. Antibodies are used for targeting due to high affinity and biological tissue-specificity. There are, however, downsides to antibody use in nanomedicine that could present issues in application moving forward: (i) Antibodies are fundamentally opsonins, a bio-recognizable signal that promotes cell-mediated uptake and clearance of foreign particles (e.g., viruses) by the reticuloendothelial system. Can we use alternative high-affinity targeting groups that would not be subjected to active biological clearance? (ii) A typical therapeutic nanoparticle (diameter ~50-100 nm) endowed with antibodies (hydrodynamic diameter of ~10 nm) would be expected to have its surface properties and function altered by addition of this bulky appendage; furthermore, there is limited area on the nanoparticle surface to attach such a large targeting group. Can we design targeting based on minimal groups that have comparable affinity while limiting impact on the properties of the functional nanoparticle? Using ultra-high affinity supramolecular interactions as a type of "molecular Velcro," our group envisions a new therapeutic nanoparticle targeting axis built on minimal small molecule affinity motifs that serve as drivers of localization, in lieu of large targeting antibodies, while at the same time not sacrificing any affinity relative to an antibody-antigen interaction. An undergraduate working on this project will be expected to learn techniques for formulating synthetic nanoparticles to contain drugs and quantifying drug release using a combination of spectroscopy and chromatography. Additionally, this individual will be tasked with validating this mechanism for targeting in vitro through microscopy of fluorescent nanoparticles on cultured cells. Students in Chemistry, Chemical Engineering, Materials Science, or Bioengineering are encouraged to apply. A minimum of some prior laboratory coursework is expected.

24. Engineering thermodynamic pathway control in peptide-based biomaterials

We are motivated to improve specificity of self-assembling peptide materials by endowing them with units that can promote a change in assembly state as a function of the presence of disease-relevant analytes and biomarkers. Typical nanocarriers for drug delivery demonstrate equilibrium-driven release. This is inefficient at best, and at worst can result in the accumulation of drug off-target in the body where it can elicit side-effects. Can we use disease-specific indicators to facilitate increased drug release specifically at the site of disease, toward non-equilibrium, responsive drug delivery? Peptide self-assembly affords one means to create nanostructures, and by virtue of these being based on non-covalent interactions, the energy barrier that must be overcome in order to induce a change in assembly state is modest relative to a system constructed covalently. Furthermore, peptide nanostructures can be designed with control over shape, interfacial curvature, and aspect-ratio. Our objective in this project is thus to incorporate analyte-sensing chemical units within a peptide backbone such that presence of the specific analyte drives a change from an assembled peptide-based drug carrier to a disassembled monomeric form accompanied by burst release of a drug. An undergraduate working on this project will be expected to learn techniques in solid-phase peptide synthesis, conduct routine characterization to study changes in material properties as a function of analyte concentration, and quantifying the loading and release of drugs from these nanostructures using a combination

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

of spectroscopy and chromatography. Students in Chemistry, Chemical Engineering, Materials Science, or Bioengineering are encouraged to apply. A minimum of some prior laboratory coursework is expected.

Department of Civil & Environmental Engineering & Earth Sciences

25. Synthesis and characterization of nanostructured electrodes for urine treatment

The influx of nitrogen from urine substantially increases the cost of wastewater treatment. Source-separated urine is becoming an ideology that presents new challenges and opportunities in water treatment and energy production. This project will focus on the development of new electrocatalysts that will target urea oxidation from urine whilst generating hydrogen gas as added value. The student will be responsible for the synthesis and electroanalytical characterization of the electrocatalysts. Though they will work with a graduate student, they are expected to have enough experience in a wet lab that they can work independently.

26. Fate and transport of engineered nanomaterials in streams

Advancements in nanotechnology will provide new solutions to challenges in food, energy, and water. To responsibly develop nanomaterials, we must gain a better understanding of the implications on environmental and human health. With increased production, nanomaterials will likely enter streams and rivers, and understanding the fate and transport of nanomaterials will be key for its responsible development. In this project, the student will conduct laboratory column and field experiments to determine the transport behavior of nanomaterials in streams. Though they will work with a graduate student, they are expected to have enough experience in a wet lab that they can work independently.

27. Synthesis of metal sulfide nano-catalysts for water treatment applications

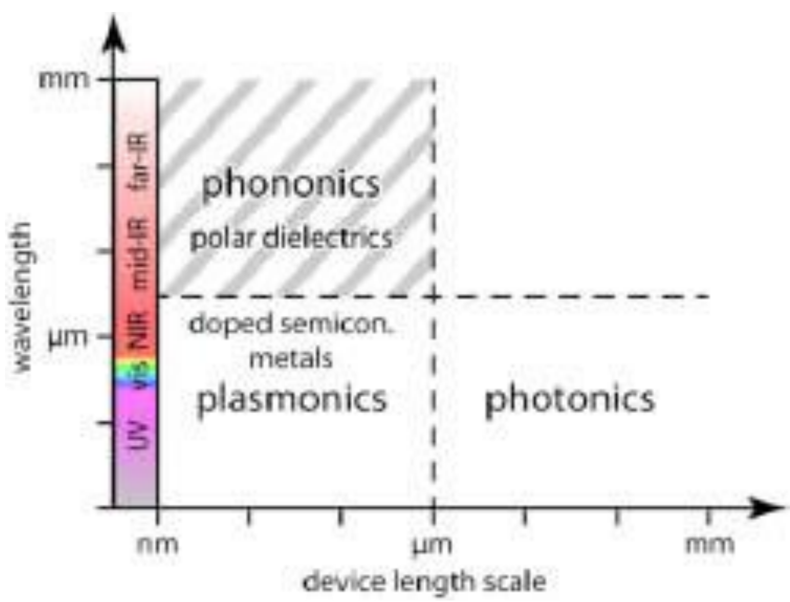
Implementation of catalytic technologies for water treatment applications has been limited by the use of non-abundant metals such as platinum. Moving toward earth-abundant elements will be key, but this poses various challenges such as reduced activity and stability. Due to unique nanostructuring and edge-site exposure, metal disulfides have the potential to replace platinum as active water treatment catalysts. In this project, the student will synthesize, characterize, and test various bimetallic metal disulfide catalysts for hydrogenation of oxidized water pollutants such as nitrate, nitrite, chlorate, and perfluorinated compounds. Though they will work with a graduate student, they are expected to have enough experience in a wet lab that they can work independently.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

Department of Electrical Engineering

28. Phononic nanoparticles for low-loss, tunable nanophotonics in the mid- and far-IR

Phononic nanoparticles are a new class of optical materials with untapped potential for realizing new mid- and far-infrared detection and sensing nanotechnologies that are functionally analogous to ultraviolet and near-infrared plasmonic nanotechnologies but with even greater sensitivity. Phononic nanotechnologies have potential application in analytical chemistry, biomedicine, environmental science, homeland security, astrophysics, and geology. However, basic scientific knowledge of the governing structure-property relationships for engineering the optical properties of phononic nanoparticles are not well understood or developed. Therefore, students on this project will investigate the optical properties of candidate phononic materials using both modeling and experimental characterization of synthesized nanoparticles. As such, this interdisciplinary research experience will cut across both materials science and optical science.

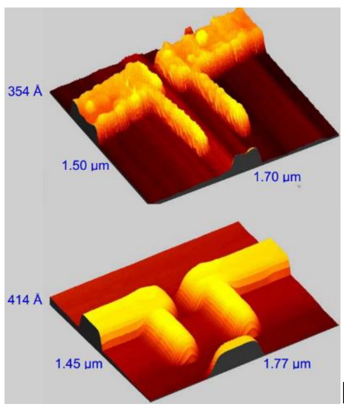


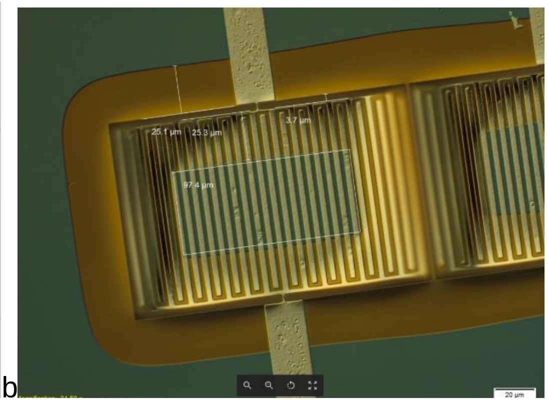
29. Probing piezo- and ferro- electrics with a nanoprobe

The phenomenon of ferroelectricity (FE) – the ability of a material to have a spontaneous electric polarization that can be reversed by the application of an external electric field – holds a promise to create multifunctional materials and devices for a variety of potential applications. Piezoelectricity (PE) – the ability of material to exert mechanical force on application of electric field – is a closely related phenomenon: all FE materials are required by symmetry considerations to be also PE. Both FE and PE have recently attracted a lot of attention in the electronic industry due to enormous progress in downscaling that made it possible to utilize these effects on the nanoscale. But how do we know that these tiny objects under your microscope are piezo- or ferro- electrics? This project is aimed at answering this question. We are going to add an extra capability to our existing nanoscale tool, a standard high resolution Atomic Force

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

Microscope Agilent 5100 (Fig a). In this project, a Piezoresponsive Force Microscope will be created and applied for characterization of PE and FE ultra thin films fabricated at Notre Dame. Projects in the group of Professor Alexei Orlov study the new types of ultra-low power logic circuits that require on-chip “power distribution centers” – piezoelectric power clocks (Fig b), and aim to produce and study high quality nanoscale FE materials by solution combustion synthesis. Over the course of this project you will learn first hand how an AFM works, including all the bolts and nuts, control circuitry, feedback loops, and lock-in amplifier techniques, and get the feel for angstrom distances. You will be making and using conductive tips and figure out how to use the phase of modulating signals to obtain information about FE and PE materials. By the end of this project we will be able to characterize PE and FE materials and create beautiful 3D images of their electrical response. Students will work on the building of the system, tip and sample fabrication, and, of course, actual imaging using the system. Experience with code writing for control programs will be very useful. Physics, Electrical Engineering, Chemical Engineering, and Computer Science students are preferred. Some knowledge of programming, data analysis and soldering is helpful.

a 

b 

a) AFM micrographs of Au (top) and Pt (bottom) single-electron transistors

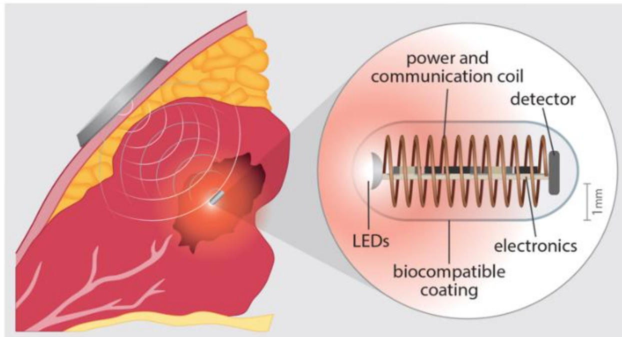
b) an optical micrograph of AlN PE clock resonator fabricated at NDNF

30. Development of microimplants for deep tissue optical sensing

Despite the explosive growth in the development of wearable and implantable sensors for monitoring health and personal wellness, there are currently no viable sensor technologies that can sense targets deep within the human body. They are limited to sensing cutaneous or shallow subcutaneous tissue volumes, have limited functionality, or are simply too large and obtrusive. This prevents their use in some of the most impactful areas of medicine including monitoring solid tumors, simultaneous deep brain sensing and stimulation, and monitoring diseases of the internal organs. The long-term goal of this project is to develop an extensible microimplant platform that can ultimately be placed anywhere in the human body and provide sensitivity to multiple biomolecular targets continuously and in real-time. This summer project will entail sensor design, modeling (mechanical and functional), and prototyping of wireless microimplants using advanced manufacturing processes. Although students of all levels will be considered, candidates should be studying electrical, mechanical, or biomedical engineering. Preference will

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

be given to candidates that have taken an optics/photonics course and/or have experience with 3D CAD modeling tools.



Department of Aerospace and Mechanical Engineering

31. High throughput spray coating of membranes for applications in desalination and waste chemical recovery

The technical objectives of this project ar to optimize and characterize a new spray coating system developed in the SST Research Lab for the high throughput processing of membranes. We have developed a piezoelectric-based spray system and developed a high throughput coating system for membranes. This research will focus on optimizing the process conditions (spray rate and duration, number of coatings, solution chemistry).

The student will conduct spray experiments and membrane characterization and draw conclusions about optimal manufacturing process in collaboration with graduate student or post-doc. Any science and engineering discipline is acceptable, although those with a background in chemistry and/or electrical engineering are preferred. The student must be willing to work primarily on experiments in a very detailed and systematic manner.

32. Electrical characterization of plasma behavior in catalyst systems

The technical objectives of this project are to characterize plasma behavior in catalyst systems using various electrical measurements. Catalyst systems such as those used for the production of synthetic gas from methane and carbon dioxide or ammonia from nitrogen and hydrogen can be enhanced by a plasma (gas discharge). This research will focus on understanding this enhancement at a fundamental level by correlating electrical behavior in the plasma to catalysis enhancement. The student will conduct plasma experiments under different conditions and take electrical measurements of the plasma behavior in collaboration with a graduate student or post-doc. Any science and engineering discipline is acceptable, although those with a background in electrical or chemical engineering are preferred. The student must be willing to work primarily on experiments in a very detailed and systematic manner.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

33. Optical characterization of plasma behavior in catalyst systems

The technical objectives of this project are to characterize plasma behavior in catalyst systems using an optical technique called optical emission spectroscopy. Catalyst systems such as those used for the production of synthetic gas from methane and carbon dioxide or ammonia from nitrogen and hydrogen can be enhanced by a plasma (gas discharge). This research will focus on understanding this enhancement at a fundamental level by correlating the light produced by the plasma to catalysis enhancement. The student will conduct plasma experiments under different conditions and take optical measurements of the plasma behavior in collaboration with a graduate student or post-doc. Any science and engineering discipline is acceptable, although those with a background in electrical or chemical engineering are preferred. The student must be willing to work primarily on experiments in a very detailed and systematic manner.

34. Design, construction and validation of a Teflon-based flow cell

Substrate-based syntheses have a significant advantage over their colloidal counterparts in that the chemical environment can be rapidly transformed by flowing heated water over an anchored substrate as a valve manifold controls the injection of various reactants into the liquid stream. Dr. Neretina's research group initiated a project that will see the design, construction, and validation of a Teflon-based flow cell. The proposed chamber, shown in Figure 1, will use a variable-flow peristaltic pump to flow reactants over substrate-immobilized seeds as the ongoing reaction is monitored spectroscopically in real-time. Initial efforts will be directed toward constructing the flow cell. Obtaining a uniform flow field is a primary objective that will be realized by inserting a shower-head-like component into the liquid stream. Its design will be based on simulations performed using the ANSYS Fluent software package and assessed by examining sample uniformity (SEM, optical spectroscopy). In situ monitoring will be used to either identify spectroscopic signatures, which indicate that a reaction is complete, or search for those that have been determined through FDTD (finite difference time domain) simulations. An undergraduate student involved in this project will assist a graduate student in the design, simulations, construction or validation of the flow cell. Background in engineering, materials science, physics or chemistry will benefit the project.

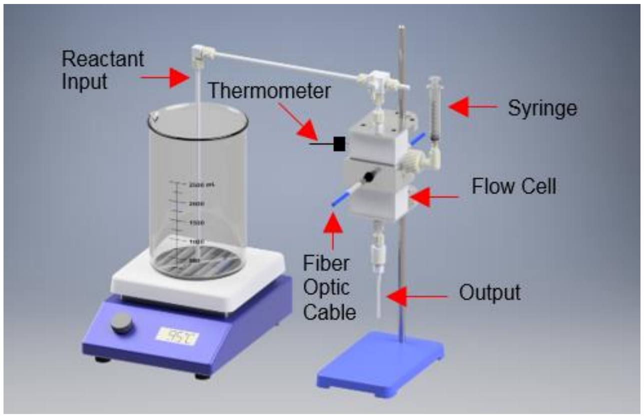
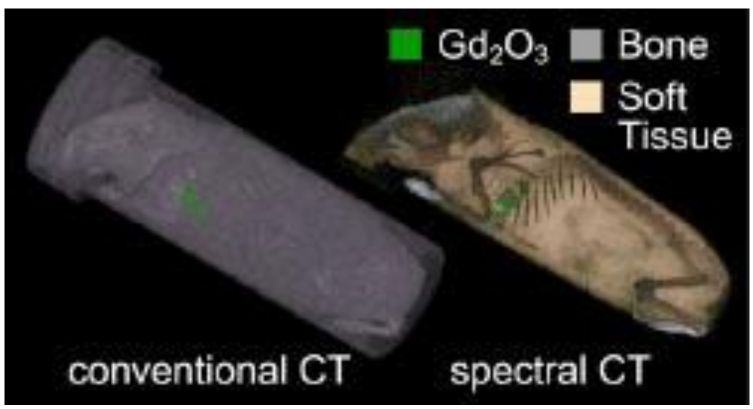


Figure 1. Proposed CAD drawing of the flow cell.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

35. Nanoparticle contrast agents for quantitative molecular imaging with CT

Molecular imaging with computed tomography (CT) could offer a single, low-cost and widely available modality for combined molecular and anatomic imaging at high spatiotemporal resolution. Nanoparticles (NPs) comprising high-Z metals, such as Au, have gained recent interest as X-ray contrast agents due to enabling the delivery of a greater mass payload compared with molecular contrast agents used clinically. Concomitant developments in photon-counting spectral CT are also transforming the capabilities of CT by providing quantitative multi-material decomposition. Therefore, students on this project will investigate the design, synthesis, and application of NP contrast agents for quantitative molecular imaging with CT. Core-shell NPs are designed for strong X-ray contrast, biostability, multimodal/multi-agent imaging, and targeted delivery. Applications include quantitative molecular imaging of multiple probe/tissue compositions, specific cancer cell populations (e.g., HER2+ breast cancer cells, cancer stem cells, etc.), tumors, associated pathologies (e.g., microcalcifications), drug delivery, and biomaterial degradation using both conventional CT and photon-counting spectral CT. Students will also interact with collaborators at the IU School of Medicine in South Bend and/or the Loyola University Medical Center in Chicago.



36. Constructing an engineered breast tissue model for mimicking breast tissue microenvironment

Breast cancer is one of the leading threats for female health. It is reported that breast tissue microenvironment was related to breast cancer risk. However, the diversity of tissue microenvironment such as the stiffness and composition of extracellular matrices (ECM), as well as the involvement of stromal cells, makes it extremely difficult to mimic this microenvironment in vitro. One method to gain more precise control over the 3D microenvironment geometry and stiffness is to use photo-reactive hydrogels. The biodegradable hydrogels with tunable composition and stiffness can provide more precise control over the tissue microenvironment, and are essential for understanding cellular responses. In this project, the students will characterize native breast tissues and construct an in vitro engineered breast tissue with hydrogels that can model the in vivo breast tissue microenvironment. Students with cell culture skills are preferred.

Note: Applicants should not contact faculty during the application phase and may be disqualified for iSURE for this reason. Please contact globalprograms@nd.edu for any questions.

#37 and #38 are for students who can participate in the 5/21 - 7/14 or 6/3 - 7/28 time frames ONLY.

2018 iSURE PROJECTS
Within the Center for Research Computing

37. Data Intensive Scientific Computing-DISC

Students in the DISC program will learn how to use high performance computing and big data technologies to enable new discoveries in computer science, physics, and biology. We work on grand challenge problems, like discovering new galaxies in digital imagery, discovering new fundamental particles, using gene sequencing to understand disease, predicting the effect of new drugs using computational modeling, and many more. To do this, we harness large scale computing clusters and big data systems composed of hundreds or thousands of machines, all working together in concert. To make advances in these areas, our goal is to train the next generation of scholars to be adept in both scientific domains and advanced computing techniques.

38. Computational Social Science REU

This Computational Social Science project is a program where ten students will work collaboratively with expert mentors and select from a wide variety of computational social science projects at the University of Notre Dame. Computational social science as an approach to analyzing the social world is has been growing rapidly. An increasing number of social interactions are taking place in the virtual world, using social media, mobile phones, and other electronic means. The digital traces of such interactions and the greater availability and detail of CSS data sets (e.g. surveys, census data, historical records) yield and exponential growth in data available for analysis. New cyberinfrastructure tools and methodologies for data analytics are needed to capitalize on this resource and enhance American economic competitiveness. This REU training environment will develop multidisciplinary social scientists with the appropriate expertise to answer the computational social science data growth challenges and opportunities.