Project Title: Synthesis and Catalysis of Bimetallic Nanocatalysts
Faculty name and email: Franklin (Feng) Tao, ftao@nd.edu
Project description:
Research of Franklin (Feng) Tao group is in the interdisciplinary field of heterogeneous catalysis and nanoscience for efficient energy conversion. We focus on nanocatalysis crucial for efficient energy harvest and conversion, chemical transformation, and environmental remediation. The goal of our research projects is to develop efficient nanocatalysis using different syntheses that build on in-situ operando studies of nanocatalysis using new analytical techniques including in-house (using Al Kα) ambient pressure X-ray photoelectron spectroscopy available in our group. Our research activity includes synthesis of nanocatalysts, measurement of catalytic performance and energy efficiency, and in-situ characterization under reaction conditions. We currently work on synthesis and catalysis in generation of hydrogen from methanol steaming reforming and partial oxidation, conversion of carbon dioxide to fuel molecules through thermal catalysis, selective production of transportation fuels from syngas, generation of hydrogen from water through photocatalysis, and catalysis toward high selectivity in environment remediation. In addition, we collaborate with a few groups by using multiple in-situ techniques including environmental TEM (ETEM) and extended X-ray absorption fine structure (EXASFS) toward a deep and fundamental understanding of nanocatalysts at molecular and atomic.
Pre-requisite courses or skills: Experience in synthesis of nanomaterials with colloidal chemistry is a plus.

Project Title: Large area Solution-Liquid-Solid growth-enabled epitaxy for low cost solar cells
Faculty name and email: Masaru Kuno, mkuno@nd.edu
Project description:
Rapid developments in the growth of low-dimensional materials (e.g. colloidal quantum dots and semiconductor nanowires) represent timely opportunities for advancing third generation solar cells that aim to transcend the Shockley-Queisser limit. This stems from their unique size- and shape-dependent properties, which open up opportunities for enhancing and even controlling charge separation at the molecular level. However, the use of chemically synthesized nanostructures is not without drawbacks. An unavoidable problem when using colloidal nanomaterials in solar cells is the presence of interfaces/heterojunctions that act as charge recombination centers. These interfaces suppress resulting device power conversion efficiencies to values below those of conventional 1^{st} and 2^{nd} generation devices. As a consequence, much effort has gone into suppressing their effects. This study begins by asking if there isn't a better way to make 3^{rd} generation devices by *avoiding* the use of chemically synthesized nanostructures. Specifically, we propose to grow large area, coherent, semiconductor nanolayers by combining the underlying principle of low cost, low temperature solution-liquid-solid nanowire growth with planar substrates. Resulting semiconductor nanolayers will be used as active materials in subsequent Schottky junction/metal-insulator-metal photovoltaics wherein the absence of interparticle junctions will boost device efficiencies. The flexibility of the approach also enables the creation of compositionally complex nanolayers, planar heterostructures and even electronically graded materials which should foster efficient photogenerated charge separation. The proposed growth strategy simultaneously leads to the creation of two-dimensional nanomaterials, enabling fundamental explorations of their thickness-dependent optical/electrical properties as well as dielectric sensitivities.
Pre-requisite courses or skills: No prior experience required.

Project Title: Capillary electrophoresis for bottom-up proteomics
Faculty name and email: Norm Dovichi (ndovichi@nd.edu)
Project description:
Bottom-up proteomics typically employs a liquid chromatographic separation of the tryptic digest of a complex protein sample, followed by electrospray ionization and tandem mass spectrometry analysis. This technology is robust and very widely employed. Nevertheless, there is a need for simpler and less expensive alternatives. This group is developing a set of electrophoretic techniques to replace liquid chromatography for bottom-up proteomics. The candidate will spend the summer evaluating capillary zone electrophoresis for the separation of tryptic peptides. The candidate will receive training in capillary electrophoresis, operation of an Orbitrap mass spectrometer, and in proteomic sample preparation and data analysis.
Pre-requisite courses or skills: Some experience in chromatography or other analytical separation method would be useful.

Project Title: Computational Design of Catalytic Materials
Faculty name and email: Bill Schneider (wschneider@nd.edu)
Project description:
Quantum mechanics provides the mathematical rules that describe the chemical properties of materials, and with modern computers it is now possible to use those rules to understand the properties of current materials and predict those of those yet undiscovered ones. In the Schneider group we use these tools to predict the behavior of catalytic materials---substances that accelerate catalytic reactions. In this project the student will learn to apply these tools to one of the problems currently being worked on in our group. These problems relate to the efficient storage and use of energy, from catalyzing the production of hydrogen fuel to capturing carbon dioxide to prevent its released to the atmosphere to cleaning up nitrogen oxides produced during combustion. The student will be paired with a graduate student or post-doc, will be trained in the use of these high performance computer codes, and will complete and present and individual project on computational materials design. More information can be found at the Schneider group website, www.nd.edu/~wschnei1.
Pre-requisite courses or skills: Desirable to have completed Physical Chemistry

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Project title: Synthesize Hyperbranched Polymers with Uniform Structure and Explore Their Application in Gene Therapy
Faculty name and email: Haifeng Gao (hgao@nd.edu)
Project description:
Recently, a new synthetic strategy is developed in our research group that successfully produces hyperbranched polymers with high molecular weight ($M_n \sim 10^6$) and uniform structure ($M_w/M_n \sim 1.2$) using a one-pot microemulsion polymerization technique. The initial success reveals a general strategy of using a discrete confined space to produce functional hyperbranched polymers with tunable molecular weights and hierarchical structures. The current project is to fully investigate the features of this robust technique and to expand its application to obtain functional hyperbranched polymers for potential application in siRNA delivery.
Pre-requisite courses or skills: List of preferred skill: Polymer synthesis and characterization

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Project Title: Storable Chemiluminescent Molecules
Faculty name and email: Bradley Smith (smith.115@nd.edu)
Project description: The goal of this research project is to invent chemiluminescent versions of a radiotracer. That is, a suite of molecules that can be stored and transported at typical kitchen freezer

temperature and then made to emit visible or near-infrared light by simply warming them to room or body temperature. These molecules have potential as biological imaging agents. They are called squaraine rotaxane endoperoxides (SREP), and they are interlocked molecules with unusual structure and photophysical properties. The student will synthesize new types of SREPs and study their properties by fluorescence, chemiluminescence, and NMR spectroscopy.
Pre-requisite courses or skills: Organic synthesis preferred.

Project Title: Resolving Energy Harvesting at the Nano and Mesoscales
Faculty name and email: Libai Huang (lhuang2@nd.edu)
Project description:
Novel nanoscale materials with unique physical properties are highly promising for applications in the next generation of solar energy conversion devices. The frontier in solar energy conversion utilizing nanoscale materials now lies in learning how to integrate functional entities across multiple length scales to create optimal devices. This challenge has initiated recent research attention on mesoscale science, aiming at creating architectures with targeted mesoscale phenomena and functionalities.
To address this new frontier, we have been developing novel ultrafast microscopy techniques to resolve multi-scale energy transfer, migration, and dissipation processes with simultaneous femtosecond temporal resolution and nanometer spatial resolution. Importantly, strategies will be developed to design functional architectures to control energy and charge flow. This research focuses on nanostructured solar energy harvesting and fuel production systems. A unifying theme of these research projects is to understand the role of individual functional components and system-wide energy flow.
Pre-requisite courses or skills: Physical Chemistry

Project Title: Radiation Damage during Macromolecular Crystallography
Faculty name and email: Ian Carmichael (carmichael.1@nd.edu)
Project description:
Radiation damage due to the photoelectrons released by X-ray absorption during crystallographic data collection at synchrotron sources continues to sharply limit the rate of successful structure solution for large biomolecular targets. Global damage leads to a systematic reduction in the intensity of diffraction spots with associated loss of achievable resolution. Specific damage to redox sensitive sites is also widespread and can cloud the assignment of biological function.
We seek to provide an understanding of the characteristic order in which this specific damage is observed to occur. Factors controlling site susceptibility will be evaluated and modeled by techniques drawn from computational quantum chemistry. Predictions will be made of distinguishing features generated in the damaged sites. Such markers can be probed by complementary spectroscopic approaches to help assess the efficacy of proposed mitigation strategies.
Pre-requisite courses or skills: Quantum Chemistry

Project Title: Catalytic Approaches to NO2 activation
Faculty Name and e-mail: Seth Brown (Seth.N.Brown.114@nd.edu)
Project description:
Nitrogen dioxide is an abundant an inexpensive gas that is surprisingly gentle in its reactivity toward most organic compounds. This project involves exploration of possible transition-metal catalyzed approaches to activating NO2 for selective functionalization of organic compounds. Possible targets include transformation of boronates into nitro compounds and ligand directed nitration of C-H

bonds. Approaches to be taken include combinatorial as well as mechanistically-directed strategies for finding and optimizing possible catalytic systems.
Pre-requisite courses or skills: Two semesters of organic chemistry and corresponding laboratory.

Project Title: Development of catalysts for the activation of Carbon Dioxide
Faculty Name and e-mail: Ken Henderson (khenders@nd.edu)
Project description:
Polycarbonates are an economically valuable class of polymer, yet the traditional synthesis of these materials utilizes phosgene and produces toxic gases making this process environmentally unfriendly. More recent advances have been able to utilize 'waste' carbon dioxide; however, these processes often use environmentally and biologically harmful metals (Co, Cr, Sn) and fail to achieve high turn-over numbers (TONs). This would be very attractive from an energy perspective as CO_2 generated by fossil fuel utilization could become a useful starting material for a value added product. Thus, this would help offset some of the costs for CO_2 separation processes, in turn making these more economically viable. We have initiated a new project in our laboratory to investigate the use of s-block metals (Li, Na, K, Mg, Ca) as a replacement for the mentioned toxic and costly metals. The light *s*-block metals are biologically and environmentally begin; additionally, these metals are earth-abundant, making them cost effective alternatives. In addition, these metals offer a gradated palette of physical and electronic properties, allowing tremendous control over the fine tuning of the catalysts.
Pre-requisite courses or skills: None
