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#### DANIEL DOWLING

We primarily use X-ray Crystallography and biochemical techniques to study the structures and functions of important biological systems.

Our research focuses on two main areas:

1. *Challenging chemistry in natural product biosynthesis.* We are particularly interested in heterocycle formation within nonribosomal peptide synthetases and complex free-radical chemistry involved in natural product biosynthesis.
2. *Posttranslational or posttranscriptional modifying enzymes with implications in treating different diseases.* Current work focuses on kinases and metallo-deacetylases.

#### JASON EVANS

My research uses mass spectrometry to develop new methods and investigate biological processes. With the recent acquisition of a state-of-the-art LC-MS instrument, our main focus has recently shifted to quantitative proteomics. We are developing robust 2D-HPLC-MS<sup>3</sup> methods for accurately measuring differential protein expression patterns in yeast and human liver cells in response to the presence of a toxin, with the aim of mapping toxicity pathways. Another project focuses on studying the mechanism that arthropods use to harden their exoskeletons. Several catechols have been shown to serve as crosslinking agents linking protein and chitin via a complex biological mechanism, requiring multiple enzymes. We are developing proteomic methods for identifying the most common cross-linking sites on the cuticle proteins. A third thrust of our work studies the energetics of collisional dissociation of gas phase parent ions of triglycerides with ultimate aim of developing a robust method for the quantitative speciation of triglycerides in fats and oils.

#### MICHELLE FOSTER

The Foster group does surface chemistry and experimental physical chemistry. We use optical spectroscopies, such as diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), and scanning probe microscopies, such as atomic force microscopy (AFM), and combination techniques, such as a Raman microscope, to study chemical reactions and processes happening at complex interfaces. The group has three main areas of focus:

1. Green / Environmental Chemistry: surface science of metal oxide and metal impregnated nanoparticles to investigate heterogeneous catalytic processes and environmental remediation.
2. Materials Science: nanomechanical properties of novel core-shell nano/microspherical particles, and physical properties of

novel liquid-metal systems.

3. Biological Chemistry: development of biodegradable liquid metal nanocarriers as potent cancer theranostic agents.

#### JASON GREEN

Our research focuses on complex chemical and physical systems and their dynamics away from thermodynamic equilibrium. A current effort is to understand, design, and control how chemical reactions drive matter to self-organize into complex structures and dissipate energy. We are analyzing and characterizing mechanistic pathways to inform atom- and energy-efficient self-assembly of nanostructured materials with tailored properties. To develop descriptions of these emergent dynamical behaviors, we leverage seemingly distant disciplines of theoretical science and modern numerical methods informed by experiments and first principles.

#### QINGJIANG LI

Carbohydrate chemistry is an interdisciplinary field at the interface of chemistry and biology and mindsets of multidisciplinary collaboration are practiced in our research. While specialized in the chemical/enzymatic synthesis of carbohydrate molecules and methodology development, the research projects in the Li lab extend to their biological applications, especially in immunology and drug discovery. Here at UMB chemistry, the principles of green chemistry will also be integrated into our projects of methodology development.

#### ADHARSH RAGHAVAN

Research in the Raghavan Lab sits at the intersection of synthetic and physical inorganic chemistry and photochemistry. We take a combined experimental and computational approach to synthesize and characterize molecules and materials that respond to external stimuli such as light or heat. Our primary focus is on photo-switchable metal-metal (M-M) bonds: Materials with modifiable M-M interactions can exhibit variations in important properties such as reactivity, magnetism, light absorption and emission, redox potential, and conductivity. As such, being able to tune them using an external stimulus has tremendous potential in the design of 'smart' materials. We will design stable, photo-switchable bimetallic complexes, study structure-property relationships as a function of light (or heat) irradiation, and ultimately build a molecules-to-smart materials pipeline. Our secondary focus is on materials that exhibit room-temperature phosphorescence (RTP): Despite the utility of ultra-long RTP in applications such as information storage, lighting, and sensing, significant challenges remain. To tackle these, our group will take a crystal engineering approach to design emissive organic-inorganic hybrid materials of varying dimensionalities, and explore the mechanisms of various photophysical processes therein. Depending on the nature of the project, researchers are typically engaged in (1) inorganic and organic synthesis, (2) NMR, IR, Raman, UV-vis-NIR absorption and emission spectroscopies, electrochemistry and spectro-electrochemistry, and (3) computation.

#### NEIL REILLY

My research involves the generation, detection, and characterization of transient chemical species using laser spectroscopy. The

chemical systems I study are often known or thought to be important intermediates in the chemistries of interstellar space, fossil fuel combustion, and thermal biomass decomposition. Exotic, highly reactive molecules - which would be rapidly consumed in Earth's atmosphere - are produced and isolated in vacuum, where they can be probed by a suite of highly sensitive spectroscopic techniques. In concert with computational methods, the information obtained helps elucidate the electronic and molecular structures of these species and enables investigations of their roles in a wide variety of complicated chemical environments.

#### JONATHAN ROCHFORD

My research interests can be broadly described as physical inorganic chemistry with a principal focus being toward applications in renewable energy. In recent years, my group has established the tools necessary to conduct high impacting research in the fields of dye-sensitized solar cells, electrocatalytic and photocatalytic CO<sub>2</sub> reduction. A significant amount of synthesis is conducted in our laboratory to develop novel photosensitizers and catalysts with students being exposed to a diverse suite of analytical tools inherent with the multidisciplinary nature of each project, e.g. steady-state and time-resolved spectroscopies, electrochemistry, photo-electrochemistry, computational analysis. Our work toward solar energy conversion typically involves the development of non-innocent ligand and transition metal based molecular catalysts, both in condensed media and on solid oxide semi-conducting electrode supports. Through collaboration with the Department of Physics at UMB, we are also active in the development of novel molecular contrast agents for application in the growing field of photoacoustic (light-to-sound conversion) imaging for cancer diagnosis.

#### NIYA SA

Broad impacts of our research is to promote the adoption of electric vehicles (EV) and decrease the need for imported oil and gas. To pursue such goal, it requires understanding the limit of the rechargeable ion batteries and their degradation mechanisms. One major focus of our research group is to probe and elucidate in-operando chemical processes at the interfaces of high performance, low cost energy storage materials. Such fundamental research underpins the future development in battery technology. Specifically, we are trying to decipher the operational local chemistry environment at the electrode/electrolyte interface upon cycling with in-situ electrochemical techniques. Systems we explore include rechargeable Li ion battery technology, and also beyond lithium ion technologies. Another research area that our team is specialized is the development of the next generation beyond lithium ion technologies, which include: development of multivalent ion battery systems, advancement for next generation anode material and discovery of new electrolytes.

#### BELA TOROK

Our efforts focus on two major research topics:

1. *Organic Synthesis. Development and Application of New Metal Nanoparticle Based Catalysts for Organic Synthesis.*  
Develop new, environmentally benign chiral synthetic methods for biologically active compounds based on metal nanoparticle catalysts and readily available, chiral ligands (prefer-

ably natural products). Our goal is to contribute to the development of new efficient chiral catalysts.

2. *Medicinal Chemistry. Synthesis and Application of Chiral Organofluorine Compounds as Novel Therapeutics for Alzheimer's Disease.* Produce biologically active chiral compounds and explore their application for medically relevant problems.

Minor research projects, which accompany the above-mentioned major areas:

1. Chiral organocatalytic Friedel-Crafts hydroxyalkylation reactions
2. Development of polymer stabilized Pt and Pd nanoparticle catalyst
3. Organic synthesis by microwave irradiation and/or ultrasound

#### MARIANNA TOROK

Our group is interested in Physical Biochemistry and Green/Sustainable Medicinal Chemistry with emphasis on polypeptides, protein folding, protein-ligand interactions, and small molecule antioxidants. Research efforts are focused on understanding the chemical factors that govern protein misfolding and aggregation leading to amyloid formation, and how these results can be translated into biomedical applications. Further projects involve regulation of enzyme activity, biochemistry of free radicals, and development of novel bioactive compounds. For more information, please visit <https://www.umb.edu/directory/mariannatorok/>

#### WEI ZHANG

Efforts in our lab are to develop new organic synthetic methods for green chemistry and medicinal chemistry applications:

1. Organic Synthesis. Development of synthetic methods involving multicomponent reactions and free radical reactions to make diversity-oriented molecules with potential biological utility.
2. Medicinal Chemistry. Collaboration with Dana-Farber Cancer Institute and Harvard Medical School, Ohio State Medical School, Boston Children's Hospital, Brigham Women's Hospital, and Berlin Children's Hospital on the development of synthetic molecules as probes and inhibitors for drug discovery research.
3. Organocatalysis. Application of organocatalysis for asymmetric synthesis of organofluorine and related compounds.
4. Fluorous Chemistry. Our group is a leader in the development of new fluorous reaction and separation techniques for making compound libraries.

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