



THE UNIVERSITY OF
TENNESSEE
KNOXVILLE

DEPARTMENT OF CHEMISTRY

2024-2025 Seminar Abstracts

Department of Chemistry
University of Tennessee, Knoxville
1420 Circle Dr



The Department of Chemistry at the University of Tennessee, Knoxville is the oldest PhD granting department at the flagship educational institution in Tennessee. We have 26 tenure-track faculty members who represent the traditional subdisciplines of chemistry and engage in interdisciplinary research in materials chemistry, chemical physics, bio-organic chemistry, and neutron science. We have strong collaborative ties across departments at UT and with nearby Oak Ridge National Laboratory.

In academic year 2024-2025 we are pleased to offer 10 seminar options in a variety of research areas, detailed in the following pages. Each faculty member's image in the booklet links to their page on our website, where you can learn more about their research, publications, and achievements. Click the area of interest to the right to be taken to the corresponding section of this booklet.

To schedule a seminar please select 2-3 talks of interest and contact Jennifer Brown (jbrow209@utk.edu) to arrange scheduling. Seminars are available for both Fall 2024 and Spring 2025.

Available Faculty Seminars

Analytical Chemistry
Thanh Do

Inorganic Chemistry
Brendon McNicholas
Viktor Nemykin

Organic Chemistry
Joshua Baccile
Johnathan Brantley
Ben Xue

Physical Chemistry
Sharani Roy
Konstantinos Vogiatzis

Polymer Chemistry
Brian Long
Bin Zhao



Thanh Do, Analytical Chemistry
Taming Conformational Heterogeneity on Ion Race Tracks

About 85% of the human proteome is undruggable by traditional small molecules. The potential drugs must be large and flexible enough to engage large, groove-shaped binding sites, or to bind at the interface between two proteins. Cyclosporines, a class of N-methylated macrocyclic peptides, have challenged the traditional view of structure-based drug

design. Although cyclosporine A (CycA) has revolutionized the field of organ transplantation since 1983, attempts to design drugs similar to it for different targets have been unsuccessful, indicating a knowledge gap in the roles of N-methylation and the functions of conformational heterogeneity in cyclosporine chemistry. Cyclosporines are flexible due to N-methylation, and each cis/trans amide isomerization can alter the molecule's conformations and physicochemical properties. CycA can bind to multiple targets (two are known so far) with different bound states, indicating that the bound states depend on the target. Previous studies have shown that the bound states (to known targets) exist as minor conformers in solution. This suggests that cyclosporines may bind to their targets via a reversed induced-fit model, where the ligand alters its conformation to accommodate the binding sites. Therefore, the number of targets that cyclosporines can bind to is likely proportional to the number of possible conformers it can adopt. Thus, to fully understand the biochemical properties of cyclosporines, my lab has worked to accurately probe both major and minor conformers of CycA and CycA analogs, using a wide range of techniques, including both experimental (X-ray/neutron crystallography, ion mobility mass spectrometry, 2D-NMR, ion spectroscopy), and computational approaches. We discovered an intricate conformational network and dynamics modulated by divalent ions.

Read more about Thanh Do's work [here](#).



Brendon McNicholas, Inorganic Chemistry
Macrocycles and Metal Inorganic Frameworks for Energy Storage and Conversion

Conjugated macrocycles and metal inorganic frameworks are two promising architectures based on molecular building blocks. Aside from their complex and interesting electronic structures (a fundamental interest in our group), both sets of materials can readily donate or accept multiple electron equivalents. Because of this, our group is interested in leveraging

these two materials classes for a myriad of applications, including energy storage (mono- and multivalent cation battery cathodes and anodes) and photo/electrocatalysis (small molecule reduction or oxidation for sustainable upcycling). The first part of this talk focuses on the electronic structure of two classes of porphyrnoids (tert-butylated metallophthalocyanines and cyano-phenylated metalloporphyrins), Lewis acid-base effects on their electronic structure, and their potential applications in photocatalytic oxidation. The second part of this talk centers on the tuning of Prussian Blue analog frameworks and their environment for electrocatalytic oxidation reactions and for use in multivalent batteries.

Read more about Brendon McNicholas' work [here](#).



Viktor Nemykin, Inorganic Chemistry
Creating New Electron-Deficient Types of Functional Dyes That Are Potentially Useful as Electron Acceptors in Solar Cells

We have developed synthetic protocols for the preparation of several classes of electron-deficient functional dyes that have a first reduction potential close to the traditional fullerenes. These include (i) functionalization of BODIPY core at meso-position; (ii) creation and functionalization of BOPHY platform; (iii)

selective synthesis of 2-pyridone-BODIPYs; (iv) creation of electron-deficient “Manitoba Dipyrromethene” (MB-DIPY) chromophores and (v) discovery of hybrid β -isoindigo-aza-DIPY systems and/or functionalization of BOPHY platform; (iii) selective synthesis of 2-pyridone-BODIPYs; (iv) creation of electron-deficient “Manitoba Dipyrromethene” (MB-DIPY) chromophores and (v) discovery of hybrid β -isoindigo-aza-DIPY systems.

Read more about Viktor Nemykin’s work [here](#).



Joshua Baccile, Organic Chemistry
Elucidating the Role of Five Carbon Metabolism in Disease

Isoprenoids are structurally diverse metabolites with an array of critical bioactivities which include cell membrane integrity (e.g., cholesterol), glycoprotein synthesis (e.g., the dolichols), steroid hormone signaling (e.g., androgens, estrogens, and cortisol), and mitochondrial health (e.g., coenzyme Q).

Human isoprenoids derive from the mevalonic acid (MVA) pathway, whereas many plants and bacteria utilize the methyl erythritol phosphate MEP pathway. Both MVA and MEP pathways converge on the same two structurally related five-carbon precursors, isopentenyl pyrophosphate (IPP) and dimethylallyl pyrophosphate (DMAPP), which are chain extended to form higher order isoprenoids. Therefore, IPP and DMAPP are the central five-carbon precursors for all isoprenoids in all organisms. Beyond their role as precursors, IPP and DMAPP also directly modify other small molecules (ATP) and macromolecules (37A tRNA) in a process known as prenylation. Levels of IPP and DMAPP are directly involved in cardiovascular disease and have recently been implicated in cancer, cystic fibrosis, and nonalcoholic fatty liver disease. Despite this importance to human health, the mechanisms responsible for both the clinical effects observed by modulating the intracellular concentration of IPP and DMAPP and the distinct bioactivity of IPP and DMAPP are relatively poorly understood. This talk will be focused on our efforts to bridge this critical scientific gap through the development of a suite of IPP and DMAPP based chemical probes and methods for the metabolic labeling of isoprenoids and prenylated molecules. I will discuss our synthetic approach for access to a wide variety of IPP and DMAPP analogs. Currently, we are leveraging these compounds to do metabolic labeling studies, and to study the independent biochemical activity of IPP and DMAPP. Lastly, I will discuss the future of metabolic labeling in the prenylome, which is to develop methods to label isoprenoids and prenylated molecules in a cell-specific manner.

Read more about Joshua Baccile’s work [here](#).



Johnathan Brantley, Organic Chemistry
Exploring New Platforms and Methods for Soft Polymer Editing

The exploration of unique architectural elements is critical for advancing our fundamental understanding of polymer structure-property relationships and accessing next-generation materials. As such, expanding the range of functional groups that can be incorporated within polymers is paramount for developing advanced soft materials. The precise installation

of reactive motifs, in particular, could be leveraged to access tunable (or otherwise functional) polymers with bespoke properties. Here, we will explore a variety of novel materials that are decorated with underutilized functional groups in materials science. For example, cumulenes are valuable synthetic handles that are largely absent from macromolecular architectures. Metallocarbenes, which participate in numerous chemical transformations, are also underexplored functional groups in polymer chemistry. We found that both motifs could be incorporated into polymers with good fidelity, and the resultant materials exhibited various stimulus-responsive behaviors (e.g., network formation or CO release). We will also explore how new methodological developments can enable iterative modifications to realize functionalization and/or degradation of various polymers. For example, Suzuki chemistry can be harnessed to decorate polymers with reactive aryl aldehydes (which can undergo an array of subsequent modifications). Conversely, electrochemical editing of polymers (via radical cation pathways) can open new opportunities for polymer degradation and/or functionalization.

Read more about Johnathan Brantley's work [here](#).



Ben Xue, Organic Chemistry
Metal Complexes as Molecular Quantum Materials, Studies by Advanced Spectroscopies

Transition metal and lanthanide complexes with unpaired electrons are of intense current interest as molecular quantum materials. Spins of the complexes lead to single-molecule magnets (SMMs), chemical qubits (quantum bits), and Haldane topological materials with potential applications in spintronics and quantum computers. Our recent studies of

such complexes, in particular their magnetic properties, will be discussed. Advanced spectroscopies, such as far-IR and Raman magneto-spectroscopies, high-field electron paramagnetic spectroscopy (HFEPR), and inelastic neutron scattering (INS), have been used to determine magnetic excited states and spin-vibrational coupling.

Read more about Ben Xue's work [here](#).



Sharani Roy, Physical Chemistry
Understanding the Adsorption and Reactivity of Subsurface Oxygen Within a Silver Surface

Akin to the pressure gap between laboratory surface-science experiments performed under ultrahigh vacuum and industrial surface chemistry conducted under high gas pressures, theoretical models of gas-surface interactions are often developed for low gas concentrations yet applied to surface phenomena that occur under high gas concentrations. The primary

reason for this discrepancy is the steep cost of computing chemical properties at high surface concentrations (or coverages) of the gas using quantum chemical methods. To address this challenge and to study the percolation of gases just beneath the surface, i.e., into the subsurface, at high coverages, we have developed lattice-gas adsorption models that include surface as well as subsurface sites in a crystalline solid and are fully parameterized using density functional theory. We have applied the models to study the adsorption of atomic oxygen on the Ag(111) surface, first as functions of coverage and temperature using canonical Monte Carlo simulations, and next as functions of pressure and temperature using grand-canonical Monte Carlo simulations. The simulations reveal the conditions under which subsurface adsorption occurs and provide insight into how subsurface adsorbates might participate in catalytic partial oxidation on silver surfaces. Overall, our study shows that the lattice-gas adsorption model offers a simple and insightful theoretical framework to bridge the pressure gap and explore the competition between surface and subsurface adsorption in gas-surface systems.

Read more about Sharani Roy's work [here](#).



Konstantinos Vogiatzis, Physical Chemistry
From Artificial Intelligence to Chemistry: Challenges and Applications

Artificial intelligence (AI) rapidly changes many aspects of chemical sciences, from drug discovery, material design, and the discovery of new reactions and molecules till the acceleration of computer sciences and robotics for chemical applications. In my talk, I will cover key aspects of AI and modern chemoinformatics including molecular representations and descriptors,

virtual screening of databases for molecular and material discovery, and machine learning for computational chemistry. Representative examples from the research activities of our group will be discussed, such as the automated search of molecules with strong binding of CO₂, exploration of polymer properties, and the design of new molecular catalysts.

Read more about Konstantinos Vogiatzis' work [here](#).



Brian Long, Polymer Chemistry
Teaching Old Chemistry New Tricks to Address Modern Challenges in Chemistry and Biology

The Long Research Group utilizes the tools of organic synthesis, polymer science, and organometallic chemistry to address interdisciplinary challenges within the fields of macromolecular (polymer) chemistry and catalyst design. Our research projects are often fundamental in nature, but aim to tackle research problems and topics with real-

world implications extending well-beyond the academic laboratory. Over the past several years, our research group has led advancements in olefin polymerization catalyst design, ring-opening polymerization catalysis, and tailored gas separation membranes. While these research areas have been fruitful, both in terms of research progress and student training, the Long Research Group has recently welcomed several new research projects into our expanding research portfolio. These projects aim to address current limitations within the field of polymerization catalysis and deepen our fundamental understanding of biological systems. More specifically, this talk will highlight our efforts to: a) develop a new polymerization methodology, termed photoinduced olefin polymerization (PIOP), that may provide the enabling chemistry required to 3D print polyolefins directly from monomer, and b) harness amphiphilic copolymers to efficiently and selectively extract integral membrane proteins for structure elucidation and function studies.

Read more about Brian Long's work [here](#).



Bin Zhao, Polymer Chemistry
Macromolecular Brush Materials: From Science to Applications

Macromolecular brush materials are composed of polymer chains densely grafted by one end on a solid substrate, commonly called polymer brushes, or on a polymer backbone, descriptively named molecular bottlebrushes (MBBs). Characterized by the stretched, deformed conformations of end-tethered polymer chains, these brush materials have found applications

in numerous areas, including surface-responsive materials, antifouling, lubrication, drug delivery, advanced nanocomposites, and emulsifiers. In this talk, I will first introduce the basic chemistry for the synthesis of surface brushes and bottlebrush polymers and then present three types of brush materials from our research: (a) multivalent hairy nanoparticles (NPs), (b) oil-soluble brush NP lubricants, and (c) stimuli-responsive MBBs. By growing two distinct polymers from the surface of 20 nm NPs, we show for the first time the fabrication of multivalent brush NPs with a small but defined number of nanodomains from microphase separation of mixed brushes, which opens up a new avenue for the metamaterial fabrication. While inorganic NPs are potentially effective oil lubricant additives for friction and wear reduction, further development is hindered by their poor stability in hydrophobic oils. By synthesizing oil-soluble polymer brushes from metal oxide NPs, we demonstrate that such brush NPs exhibit superior stability in polyalphaolefin oil and significant reductions in friction and wear are achieved. In the third work, well-defined stimuli-responsive multicomponent MBBs are synthesized by "click" reactions. These brush molecules can undergo reversible shape transitions between wormlike/starlike and collapsed yet stable globular conformations in response to external stimuli. We show that stimuli-responsive MBBs are efficient and robust emulsifiers, exhibiting the properties of both inorganic particle and flexible polymer surfactants.

Read more about Bin Zhao's work [here](#).

For More Information

Department of Chemistry

1420 Circle Dr

Knoxville, TN 37996

865-974-8019

jbrow209@utk.edu

chem.utk.edu
