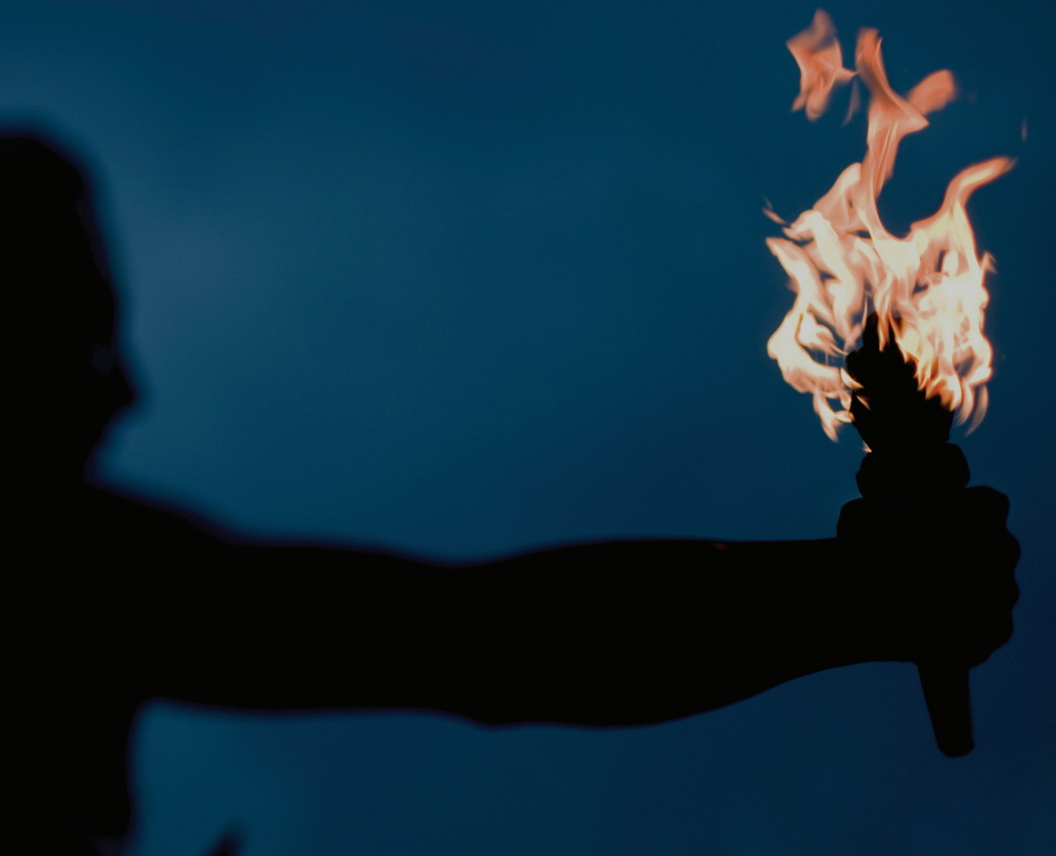
THE UNIVERSITY OF TENNESSEE KNOXVILLE
DEPARTMENT OF CHEMISTRY

2025-2026 Seminar Abstracts

Department of Chemistry
University of Tennessee, Knoxville
1420 Circle Dr



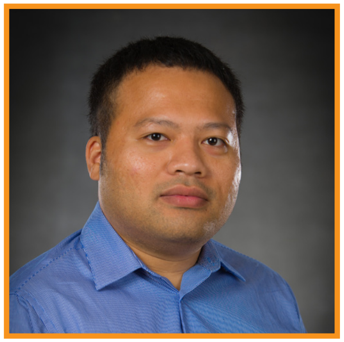
The Department of Chemistry at the University of Tennessee, Knoxville is the oldest PhD granting department at the flagship educational institution in Tennessee. We have 28 tenure-track faculty members who represent the traditional subdisciplines of chemistry and engage in interdisciplinary research 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 2025-2026 we are pleased to offer 11 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.

Available Faculty Seminars

Learn more about Chemistry at UT at chem.utk.edu



Thanh Do, Analytical Chemistry

Seminar 1:
Duplicated Insulin Genes: Proteoforms, Isoforms, and the Fine Line Between Nature's Errors and Ingenious Design

Mouse and rat models are staples of diabetes research, but are they the right choice? Unlike humans, which have a single insulin gene, mice and rats possess duplicated insulin genes (Ins1 and Ins2), producing two distinct insulin proteins. Previous studies suggest Ins1 is defective while Ins2 offers protection against diabetes—an intriguing paradox that remains poorly understood. Decades of research have overlooked the differential responses of these murine insulin isoforms to diabetic conditions, largely due to the lack of effective analytical tools for isolating and characterizing Ins1 and Ins2 from mouse islets. In 2019, we addressed this challenge by pioneering an analytical method combining nanoflow liquid chromatography (LC) with ion mobility spectrometry-mass spectrometry (IMS-MS), enabling the analysis of as little as one-tenth of a single mouse islet. This approach not only quantifies isoform-specific insulin secretion and total levels but also provides critical insights into their structures, biochemical properties, and posttranslational modification tendencies. Moreover, we uncovered a novel link between pain peptides elevated in headache disorders, such as migraines, and their regulatory effects on insulin, offering new avenues for understanding the intersection of metabolic and neurological diseases.

Seminar 2:
Toward the Design of Membrane-Permeable Macrocyclic Peptides for Undruggable Targets: A Biophysical Chemistry Perspective

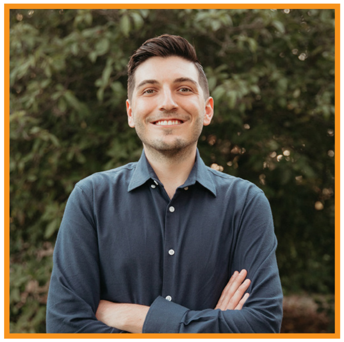
About 85% of the human proteome is undruggable by traditional small molecules. The potential drugs must be large and flexible enough to engage large, groove-shaped binding sites, or to bind at the interface between two proteins. Cyclosporines, a class of N-methylated macrocyclic peptides, have challenged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

Yingwen Cheng, Analytical Chemistry
Routes Towards Stronger Batteries: Materials, Electrolytes and Interfaces

The adoption of sustainable electricity in transportation and power grids requires advanced batteries that are cheaper, safer and more reliable compared with the state of the art, the buildings of which are deeply rooted in innovations in novel materials as well as mechanistic understandings on the synthesis, transformation and stabilization of these materials under electrochemical potentials. This presentation will discuss routes and challenges towards next generation batteries, followed by elaborations of our research efforts on developing and understanding novel electrode and electrolyte materials with examples from systems that incorporate metallic Li, Na and Zn as high energy anodes. Our program towards practical lithium-sulfur batteries and rechargeable aqueous Zn-MnO2 batteries will be presented.

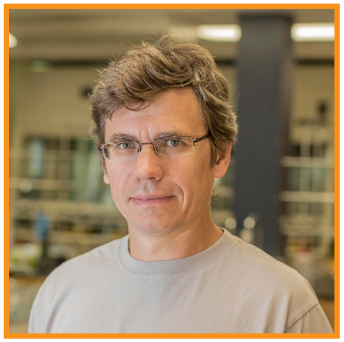
Read more about Yingwen Cheng's work **here**.



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 Funcitonal 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**.

Joseph Clark, Organic Chemistry
Precision Labeling of Small Molecules

Despite the tremendous utility that precisely deuterated small molecules have in chemical research and the development of new medicines, methods to selectively incorporate this isotopic label into molecular scaffolds are lagging. Not only is highly selective deuterium labeling challenging, but spectroscopic techniques to support advances in selective labeling reaction discovery are sometimes inadequate. Catalytic transfer deuteration and hydrodeuteration reactions are uniquely equipped to precisely install deuterium into small molecules. New copper-catalyzed reactions for the selective transfer deuteration and hydrodeuteration of alkene and alkyne-containing small molecules will be discussed along with novel spectroscopic techniques for the analysis of isotopic products.

Read more about Joseph Clark's work **here.**

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

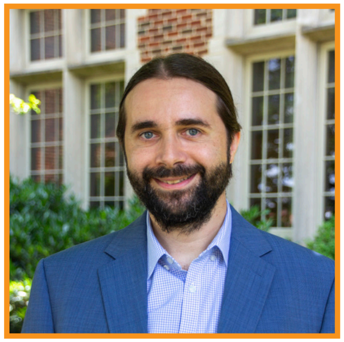
The exploration of unique architectural elements is critical for advancing our fundamental understanding of polymer structure-property relationships and accessing next-generation materials. As such, expanding the range of functional groups that can be incorporated within polymers is paramount for developing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

Sharani Roy, Physical Chemistry
Understanding Surface and Interface Chemistry from the Bottom Up Using Modeling and Computation

Surface chemistry is ubiquitous in both natural phenomena such as melting of ice, discoloring of fruit, rusting of metal and weathering of rocks, and modern technologies such as heterogeneous catalysis, solar cells, nanolithography, and microelectronics. Elucidating these phenomena requires a fundamental understanding of chemical interactions at the interface between two phases, gas-solid, liquid-solid, or gas-liquid. Theory and computation can play a powerful role toward achieving that goal by enabling us to model the individual steps of a complex surface process and study interfacial interactions at the atomic level. Here, I present two of my group's research endeavors, first, in modeling adsorption, the process in which atoms or molecules of a gas bind to the surface of a solid, and second, in modeling molecular junctions, hybrid molecule-metal systems that act as nanoelectronic components, such as resistors and diodes, and quantum devices, such as molecular switches and sensors. In the first project, we developed lattice-gas models to study the surface and subsurface adsorption of atoms on a crystalline metal over a wide range of surface concentrations or "coverage". Combining this model with Monte Carlo simulations, we determined how the surface oxidation of silver evolves with oxygen coverage and how the varying adsorption behavior influences catalytic partial oxidation reactions on silver surfaces. In the second project, we performed ab initio molecular dynamics simulations to calculate conductance distributions of single-molecule junctions and to understand how motions of the molecule, electrode atoms, and interface control conductance values and fluctuations.

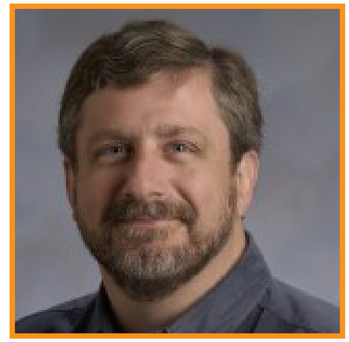
Read more about Sharani Roy's work **here**.



Konstantinos Vogiatzis, Physical Chemistry
AI-boosted Molecular Discovery: CO2-philicity, Drug Design, and Beyond

Artificial intelligence (AI) and machine learning (ML) have become important tools for chemists, enabling the analysis of vast chemical datasets. A key to harnessing these methods lies in translating molecular information into computationally useful representations, which are critical for training robust ML models. We have developed novel molecular fingerprinting methods based on algebraic topology which provide a unique perspective on molecular geometry, enhancing both the accuracy and interpretability of computational models. In this talk, I will outline the theoretical foundations of persistent homology and its adaptation for molecular applications. Representative applications related to carbon capture, drug discovery, polymer informatics, and catalyst design will be provided. This framework exemplifies the synergy between topology and AI, offering new avenues for chemical discovery and advancing our understanding of molecular systems.

Read more about Konstantinos Vogiatzis' work **here**.



Mark Dadmun, Polymer Chemistry
Developing New Feedstocks for Polymeric 3D Printing from Fundamental Principles

3D Printing has emerged as an interesting fabrication technique for models, prototypes, and complex structures. However, the range of materials that are available as feedstocks for 3D printing is limited due to the complex thermal and shear histories that the material is exposed to during the printing process. To address this problem, our group has focused on understanding and controlling scalable processing methods that use liquid-liquid phase separation to create polymer powders for Polymeric Powder Bed Fusion (PPBF), a promising and growing 3D printing technology. In this presentation, I will discuss work in our group that providing fundamental insight into the powder formation process, to offer guiding principles to design suitable precipitation protocols for a broad range of polymeric materials. Initial studies clearly show that droplet coalescence governs the powder formation process in creating polypropylene powders. (J. Polym. Sci, 62, 2605). However, expansion of this protocol to other polyolefins, such as high-density polyethylene (HDPE), emphasizes the importance of balancing the competition between precipitation of the polymer and the crystallization of the polymer from solution.
Thus, the time evolution of the solution as it goes from the cloud point temperature down to the crystallization temperature defines the thermodynamic trajectory that governs powder formation. With this guiding principle, processing protocols have been developed to create powders that are suitable for powder bed fusion from polymer blends, various grades of high-density polyethylene, and polymers from the waste stream, including PET water bottle, HDPE milk jugs, and PP pill bottles. This latter source provides a highly efficient potential process to effectively upcycle plastics in the environment

Read more about Mark Dadmun's work **here**.

Polymer Chemistry

Bin Zhao, Polymer Chemistry
Macromolecular Brush Materials

Macromolecular brush materials feature densely, covalently end-grafted polymer chains, either on a flat or curved substrate (surface brushes) or on a polymer backbone (molecular bottlebrushes). Characterized by the stretched, deformed conformations of tethered polymer chains, this unique class of polymeric materials has found applications in numerous areas, ranging from antifouling to lubrication, water treatment, drug delivery, 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 applications of brush materials from our research: (a) oil-soluble brush nanoparticle (NP) lubricants, (b) polyelectrolyte brush NPs for water treatment, and (c) stimuli-responsive bottlebrush emulsifiers. While inorganic and metal 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 show that these brush NPs exhibit a superior stability in polyalphaolefin oil and significantly reduce the friction and wear when used as an oil additive. Many oxyanions, such as ClO_4^-, ReO_4^-, and TcO_4^-, are toxic and highly soluble in water, posing significant threats to health and environment. Utilizing the principles of chaotropic ion pairing and chaotropic effect, we have designed and synthesized cationic polyelectrolyte brush NPs; these brush NPs efficiently adsorb toxic oxyanions from water and show promise in water treatment. In the third work, well-defined stimuli-responsive multicomponent MBBs are synthesized by “click” reactions. These shape-changing bottlebrush molecules are efficient, robust, and responsive emulsifiers, exhibiting the properties of both inorganic particle and flexible polymer surfactants.

Read more about Bin Zhao’s work **here.**

For More Information

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