THE UNIVERSITY OF TENNESSEE KNOXVILLE

DEPARTMENT OF CHEMISTRY

FACULTY RESEARCH

Department of Chemistry
University of Tennessee, Knoxville
1420 Circle Dr

FACULTY RESEARCH

WELCOME

The Department of Chemistry at the University of Tennessee, Knoxville supports research interests that include the traditional disciplines of chemistry and beyond. Our nationally and internationally recognized faculty members engage in cutting-edge research with real-world applications. Many of them are active in more than one research division, a testament to the department's emphasis on interdisciplinary and collaborative scientific research.

ABOUT UT CHEMISTRY

Our department is the oldest PhD granting department at the flagship educational institution in Tennessee.

Research in the department includes the 5 traditional disciplines of chemistry, as well as a number of interdisciplinary areas. Faculty members are often engaged in research that spans multiple disciplines and leverages collaborations across the university and beyond.

Our research is supported by state-of-the-art facilities and equipment, and several departmental service shops, including machining and glass blowing.

Analytical Chemistry

Tessa Calhoun
Shawn R. Campagna
Yingwen Cheng
Ziying (Nancy) Lei
Bhavya Sharma
Ziling (Ben) Xue

Inorganic Chemistry

Sheng Dai
David Jenkins
Brendon McNicholas
Viktor Nemykin
Ziling (Ben) Xue

Organic Chemistry

Joshua A. Baccile
Michael D. Best
Johnathan N. Brantley
Joseph Clark
Shawn R. Campagna
Ampofo K. Darko

Physical Chemistry

Sayan Banerjee
Thanh Do
Janice Musfeld
Sharani Roy
Konstantinos Vogiatzis

Polymer Chemistry

Mark Dadmun
Mike Kilbey
Brian K. Long
Alexei P. Sokolov
Bin Zhao

FACULTY RESEARCH

Joshua A. Baccile, Assistant Professor
Our scientific endeavors are primarily split between two main areas: 1) Developing chemical tools to investigate the production and regulation of biologically important small molecules; 2) Leveraging the engineering potential of artificial proteins to create soft materials with unique structural, functional, and diagnostic capacities. Central to our research effort will be a multidisciplinary approach, integrating expertise from protein engineering, chemical biology, cell biology, and analytical chemistry. We aim to foster a group culture where students and postdocs can enjoy collaborative research, intellectual freedom, financial support for both research and travel, and professional development for careers in academia, industry and less conventional choices.

Sayan Banerjee, Assistant Professor
The Banerjee Group aims to drive breakthroughs in energy-efficient technologies and advances chemical theory, contributing to global sustainability efforts. We work at the intersection of theoretical chemistry, machine learning (ML), and materials science. Our research focuses on (a) the electrification of the chemical industry, (b) sustainable recycling processes, and (c) quantum materials. To address challenges in these fields, we develop novel chemical theories, mathematical representations compatible with ML algorithms, and ML force fields. Additionally, we focus on creating chemistry-informed machine learning models to expand the materials design space for various applications. These applications range from catalysis to the realization of novel quantum processes in optoelectronics. Group members will gain expertise in developing chemical theory, computational chemistry and materials science methods (such as DFT and molecular dynamics), and state-of-the-art AI/ML algorithms.

Michael D. Best, Professor
Research in the Best group entails bio-organic, synthetic organic, medicinal and supramolecular chemistry. This generally involves the design, synthesis and study of organic molecules for applications pertaining to biological systems. Our lab has a particular emphasis on lipid membranes, which are at the forefront of biomedical research since lipids control critical biological pathways relevant to disease, and are beneficial for applications such as drug delivery. One area of research in the group involves the development of smart liposomes for drug delivery through the design of responsive lipid structures. Additionally, we develop functionalized lipid probes that can be applied to elucidate the roles of lipids in biological processes. These projects utilize synthetic organic chemistry to access designer lipid targets, followed by biological and analytical chemistry studies to study and apply these compounds.

Johnathan Brantley, Assistant Professor
Research efforts in the Brantley group focus on addressing chemical problems at the interface of materials science and synthetic methodology. Specifically, we envision new strategies for transforming reactive species into materials or chemical scaffolds that are challenging synthetic targets. We are particularly interested in accessing functional polymers that exhibit tunable structures and physical properties. The development of novel organometallic species, and investigating their applications in both synthesis and materials science, is another exciting area of focus. Our program integrates elements of physical organic chemistry, polymer science, synthesis, and organometallic chemistry to address both fundamental and applied problems. As such, the group's interdisciplinary approach to discovery provides burgeoning scientists at all stages of career development with an invaluable skill set.

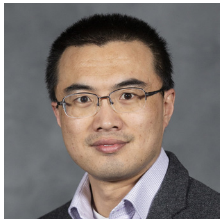
FACULTY RESEARCH

Tessa Calhoun, Associate Professor

The Calhoun lab's interdisciplinary research program specializes in the application and advancement of nonlinear spectroscopy and microscopy techniques for the study of a variety of complex systems. The overarching goal in all of our work is to understand the role of environmental effects by probing electronic excited states with a specific focus on imaging dynamic interfaces. To this end, we are currently employing optical techniques such as second harmonic scattering and microscopy to probe how living bacterial membranes uptake, transport, localize and efflux small molecules, including antibiotics.

Shawn R. Campagna, Professor, Scientific Director of UT-ORII

Research in the Campagna Group utilizes bioanalytical mass spectrometry and organic synthesis to both develop analytical tools and to probe biological phenomena, with a specific focus on understanding signaling systems and their links to metabolism. The organic group in the Campagna lab focuses on the synthesis of biologically relevant compounds, The largest of these initiatives is an ongoing collaboration with Dr. Jason Collier at Pennington Biomedical Research Center, aiming to design and synthesize novel glucocorticoid analogues that maintain their anti-inflammatory properties while minimizing their potential to induce unwanted side effects, such as steroid induced diabetes. While the analytical group is involved in a wide array of collaborations, one of the main focuses has been to understand the small molecule produced by the gut microbiome as these regulate our overall health.



Yingwen Cheng, Assistant Professor

Our research aims to develop new chemical principles to explain and control electrochemical processes for inter conversion of electrical and chemical energy. Outcomes of our work contribute to electricity-driven chemical manufacturing and storage of renewable electricity for transportation and smart power grid. We are especially interested in studying well-defined materials with systematically tunable variables to extract fundamental insights. Major topics for the near future include: 1) solid active motifs design for electrocatalytic conversion of small molecules; 2) new electrochemical interfaces for extreme batteries; 3) new ways to modulate electrochemical processes via external forces and 4) synthesis of novel nanostructures with predictable functions.

Joseph Clark, Assistant Professor

The Clark laboratory is engaged in Synthetic Organic Chemistry research. We also perform research in the areas of Pharmaceutical Chemistry, Organometallic Chemistry, and Medicinal Chemistry. We actively pursue the development of novel synthetic techniques to precisely deuterate small molecules. This area has significant implications in the development of new and safer small molecule drugs. Our reactions are currently being used to develop new drugs and study the metabolism of existing drug molecules. We are now expanding our research interests to the field of radiolabeling of small molecules. The Clark Lab is supported by several prestigious major grants, including the NIH ESI MIRA, NSF CAREER Award, and ACS PRF. Research in the Clark Lab has attracted the interest of pharmaceutical companies and we have ongoing collaborations with AstraZeneca and Vertex Pharmaceuticals. We also collaborate with the Atomic Commission (CEA) in Paris-Saclay, BrightSpec Inc., and several world-renowned academic research labs. Graduate students will have the opportunity to participate in these collaborations by working on-site at Vertex Pharmaceuticals (Boston, MA, USA), AstraZeneca (Gothenburg, SWE) and CEA (Paris, FRA).

FACULTY RESEARCH

Mark Dadmun, Professor, UT-ORNL Joint Faculty
The research in our group utilizes a variety of techniques to examine methods by which the properties of polymer mixtures can be optimized by control of dispersion size or by the selective migration of a polymeric additive to the surface. For instance, the dispersion of nanoscale particles or domains in a polymer matrix can lead to nonlinear enhancement of a variety of properties. Our group has developed an understanding of how manipulation and control of the structure of polymeric components can be utilized to efficiently and reproducibly disperse nanoscale domains (or particles) in a host polymer matrix, which can readily lead to nonlinear enhancement of material properties such as dimensional stability, flame resistance, and mechanical properties. We have also developed techniques to characterize the impact of specific branched architectures on the dynamics of a surface segregation process, the final surface structure and functionality, and the material properties of a surface-modified polymeric material. Thus, our research provides specific fundamental information to enable the design of multicomponent polymeric materials with such properties as self-healing chemical and flame resistance or hardness, exceptional impact strength, outstanding tensile properties, and dimensional stability.

Ampofo K. Darko, Assistant Professor
Research interests of the Darko group lie at the interface of organic and inorganic chemistry. We take inspiration from nature by studying selective and efficient enzymatic processes and applying these concepts in the areas of catalyst design. Recently, our group has focused on developing ligands to enable efficient and selective dirhodium(II,II) complexes for organic transformations and sensing applications. This focus has led to ligand design advancements for dirhodium(II,II) paddlewheel catalysts in carbene transfer reactions and in the detection of organophosphate nerve agents. Students in the Darko group develop competencies in organic synthesis, organometallic chemistry, and analytical chemistry. Our research endeavors have also led to collaborations with researchers at other academic institutions, government agencies, and NSF Centers for Chemical Innovation.

Sheng Dai, Professor, UT-ORNL Joint Faculty
Sheng Dai's research endeavors center on synthesizing and characterizing functional materials tailored for energy-related applications. Presently, our team is engaged in three core inquiries: (1) Catalytic Materials; (2) Separation Materials; (3) Electrical Energy Storage Materials. Our ongoing research concentrates on synthesizing and characterizing porous materials, nanoparticles, molten salts, ionic liquids, and integrated carbon-ionic liquid systems. We employ a range of synthesis techniques, including high-temperature colloidal synthesis, templating synthesis, atomic layer deposition, and solvothermal synthesis.

Thanh Do, Assistant Professor
My research combines ion-mobility mass spectrometry (IM-MS), mass spectrometry imaging (MSI), and computational modeling to bring a chemical physics outlook to problems of broad chemical interest. The overarching aims of my research are two-fold. The first is to develop fast and sensitive MS-based techniques and biophysical methods suitable for simultaneously assessing and predicting the structure, topology, composition and dynamics of exotic species in the gas phase. These species include small molecules, peptides and proteins in complex mixtures and volume-limited samples. The second overarching aim is to use these techniques for biological applications.

FACULTY RESEARCH

David M. Jenkins, Professor

The Jenkins group focuses on inorganic and organic synthesis to develop chemical systems ranging from homogenous catalysis, to porous frameworks, to surface modifications. We concentrate on three distinct areas of research, all of which are centered around the use of five-membered N-heterocycles (azoles) as ligands for transition metals. The first area is focused on developing macrocyclic tetra N-heterocyclic carbene (NHCs) ligands to stabilize metal-ligand multiple bonds for oxidative group transfer reactions. Typical catalysis studies concentrate on aziridination or epoxidation. In the second area, we utilize triazoles for the development of new metal-organic nanotubes (MONTs). These novel materials are studied on the bulk and nanoscale. The third area employs NHCs as ligands for metal surfaces of nanoparticles. These coated materials have many potential applications in medicine and electronics. To characterize the broad spectrum of compounds and materials that we synthesize, we apply a wide variety of analytical techniques including nuclear magnetic resonance and other spectroscopies, mass spectrometry, porosity measurements, and X-ray diffraction, including both powder and single crystal.

Ziying (Nancy) Lei, Assistant Professor

The Lei Laboratory leverages advanced spectroscopic and microscopic techniques to study atmospheric particles and their effects on air pollution and climate change. Addressing the challenge of these particles' complex nature, including their size (1 nm to 100 μm), acidity, diverse shapes, and chemical makeup, is crucial. These properties can continuously evolve through heterogeneous and multiphase chemistry. Using cutting-edge spectroscopy, the Lei Group aims to uncover the fundamental physicochemical attributes of atmospheric particles and their implications for the environment. Our work focuses on understanding how aerosol features like acidity, ionic strength, and size influence ice formation; enhancing molecular insights and developing methods to assess single particle characteristics and ice nucleation efficiency; and investigating how particles' physical states and morphology affect ice nucleation processes. Through this, we aim to contribute significantly to the understanding of atmospheric particles, thereby informing strategies for mitigating air pollution and climate change.

Mike Kilbey, Professor

The principal area of Professor Kilbey's research is surface and interface engineering using soft materials. We focus on studying the intrinsic links between assembly, structure and properties of ultrathin polymer films at surfaces and of molecular assemblies in solution. Our challenge is to understand the design rules whereby controllable, precise syntheses coupled with the ability to manipulate molecular assembly and intermolecular interactions lead to new and useful structures, properties, and products. We use a variety of characterization methods to probe structure and interactions on length scales approaching molecular dimensions, including surface forces measurements and neutron reflectivity, and we also use in situ ellipsometric measurements to track dynamics of assembly and changes in solvated structure of surface-tethered polymer thin films.

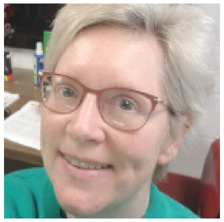
Brian K. Long, Professor

Research in the Long Group is highly interdisciplinary, utilizing the tools of organic synthesis, polymer chemistry, organometallic design, and even polymer science and engineering to address fundamental problems with real-world impact. Our research is divided into two main themes: (1) the design and synthesis of functional polymeric materials, and (2) the development and utilization of next-generation polymerization catalysts. Within those two thrusts, we have multiple research projects that aim to advance scientific knowledge within the fields of olefin and ring-opening polymerization catalysis, renewable materials, polymeric membranes for separations, 3D printing, and structural protein biology, as well as efforts to tackle the plastics waste crisis facing the world today.

FACULTY RESEARCH

Brendon McNicholas, Assistant Professor

The McNicholas lab uses spectroscopic and electrochemical techniques to develop and characterize next-generation energy conversion and storage technologies. We are particularly interested in two promising energy storage architectures: (1) Mono- and multivalent cation batteries employing metal inorganic framework cathodes and anodes, and (2) Non-aqueous redox flow batteries employing homogeneous or heterogeneous multi-electron transfer electrolytes. Additionally, the development of more efficient and stable catalysts for small molecule reduction and oxidation, specifically those related to photoelectrochemical water oxidation, fuel cell technology, CO_2 reduction, and N_2 fixation, is an active area of research. Finally, our group is also interested in the fundamental electronic structure of porphyrinoids and charge transfer complexes.



Janice Musfeldt, Professor

The overall objective of our research program is to explore the chemistry and physics of quantum materials. We employ a variety of spectroscopic methods to reveal the properties of these systems, and we use different external stimuli - such as magnetic field, light, pressure, strain, and confinement - to tune and control these properties. The goal is to discover new states of matter or physical phenomena and, at the same time, to uncover properties of technological relevance. Current research directions include (i) unraveling coupling processes in multiferroics, (ii) uncovering functionality from enhanced spin-orbit coupling and ultra-low symmetry in 4- and 5d-containing materials, (iii) revealing pressure-tmperature phase diagrams of chalcogenides, and (iv) controlling the response of nanoscale materials, interfaces, and defect structures.

Viktor N. Nemykin, Professor

Our research group is interested in the design and application of functional dyes. These dyes vary from the aromatic macrocycles such as porphyrins (pigments of life) and phthalocyanines (the most common industrial blue and green pigments) to newer BODIPY and aza-BODIPY systems. Before moving to the University of Tennessee in Knoxville, we have developed a new class of the electron-deficient functional dyes ("Manitoba dipyrromethenes" or MB-DIPYs), which have a variety of potential applications. When coupled with the organometallic fragments, such as ferrocenes, these functional materials quite often reveal exciting properties (mixed-valence, electron-migration, and photo-induced electron transfer) that are potentially useful for molecular electronics, light-harvesting, redox-switchable fluorescence imaging, and bio-imaging. We are also interested in the catalytic and electrocatalytic reactions that are facilitated by the transition-metal porphyrins, phthalocyanines, and tetraazaporphyrins for water splitting and selective C-H bond activation reactions. Finally, our group is interested in the development of reliable computational protocols for the accurate prediction of the spectroscopic properties of the functional dyes.

Sharani Roy, Associate Professor

Surface chemistry forms the foundation of a wide range of technologies, such as heterogeneous catalysis, gas storage, chemical sensing, nanoscale electronics, and solar cells. It also governs natural phenomena, such as corrosion, the rusting of iron, and the weathering of rocks. The fundamental interactions governing the above mentioned processes occur between molecules and the surface of a solid. My research group develops atomistic models of the elementary steps of surface chemistry. We study the adsorption (binding), scattering, diffusion, desorption (unbinding), and reactions of gaseous atoms and molecules on solid surfaces using a combination of density functional theory (DFT), molecular dynamics simulations, and Monte Carlo simulations. Further, we explore mechanisms of energy transfer, electron transfer, and electron transport at the gas-solid interface, and model ways in which such exchange can be harnessed into useful applications.

FACULTY RESEARCH

Bhavya Sharma, Associate Professor

The interdisciplinary research in the Sharma research group focuses on probing and characterizing the underlying chemistry and physics of biological processes. The long range research goal of the group is the use of innovative Raman spectroscopic methods to create new approaches for early detection of disease (both in vitro and in vivo detection), as well as methods for chemical and biological sensing.

Konstantinos Vogiatzis, Associate Professor

Our research focuses on the development of computational methods based on electronic structure theory and artificial intelligence for describing chemical systems relevant to clean, green technologies. We are particularly interested in new methods that help us explore the atomistic effects that contribute to the separation of CO_2 from other gases. We are also exploring novel molecular and material catalysts for the synthesis of alternative fuels. Our overall objectives are to elucidate the fundamental physical principles underlying the sorption and catalytic properties of molecules and materials, as well as to assist in the interpretation of experimental data.

Alexei P. Sokolov, Professor, UT-ORNL Governors Chair for Polymer Science

Dynamics of Soft Matter; Glass transition and Polymer Dynamics, Polymers with dynamic bonds as new recyclable materials for sustainable future.
Materials for Clean Energy Technologies, including electrolytes for batteries and supercapacitors; and membranes for fuel cells and flow batteries, membranes for gas separation, CO_2 capture and water desalination.
Dynamics and macroscopic properties of multicomponent polymeric materials, including polymer nanocomposite and block-copolymers.
The role of interfacial region and properties. Dynamics and functions of proteins and other biological macromolecules.

Ziling (Ben) Xue, Professor

Our research is centered on probing magnetism of inorganic metal complexes as new quantum materials. These complexes are either single-molecule magnets (SMMs) or Haldane topological materials. SMMS are of intense interest as new data storage materials and candidates for quantum computing. Our group has studied synthesis of SMMs. We have used state-of-the-art spectroscopies to determine magnetic separations in SMMs and to probe their magnetic relaxations, two challenges in SMM research. Our work is published in, e.g., Nature Communications and Inorganic Chemistry. Haldane topological solids contain unique antiferromagnetic chains of, e.g., Ni(II) ions, bridged by ligands, with one unpaired electron at each end of the chains. These materials have been actively studied for applications in spintronics (i.e., use of electronic spin, in addition to its negative charge, in future solid-state devices) and quantum computers. We have probed Haldane materials with 2D MOF (metal-organic framework) structures, as recently published in Nature Communications.

FACULTY RESEARCH

Bin Zhao, Professor

Our research is focused on rationally designed, precisely synthesized responsive and functional polymers for advancing fundamental understanding and exploring potential applications. Current research interests include: (i) macromolecular brush materials (hairy particles/brush particles and bottlebrush polymers), (ii) stimuli-responsive nonionic, ionic, and zwitterionic polymers, (iii) polymer adsorbents for removal of toxic persistent oxyanions from water for water treatment, and (iv) chiral ferroelectric liquid crystalline polymers. State-of-the-art polymerization methods and organic synthesis tools are used to prepare these polymeric materials, and various characterization techniques are applied to determine their structures, behaviors, and properties. Our research involves polymer science, materials chemistry, surface and colloidal science, and environmental chemistry.

RESEARCH FACILITIES

Biological and Small Molecule Mass Spectrometry Core Facility

This facility houses 8 mass spectrometers and multiple computer workstations for data analysis. The core provides project consultations as well as analytical services from sample preparation to data interpretation.

Nuclear Magnetic Resonance Facility

The NMR facilities are equipped with 5 NMR specrometers that are used for teaching, research, and services. Four of the NMRs are Solution State instruments; one 300 MHz, two 500 MHz, and one 600 MHz. A brand new 500 MHz is dedicated to variable temperature studies, with a temperature range from negative 150 to 150 degrees Celsius.

Polymer Characterization Lab

The PCL is one of the premier academic laboratories in the world for researching novel properties of newly designed polymeric materials. The characterization equipment provides information on polymer properties from the molecular scale to macroscopic, as well as structural and flow properties.

X-Ray and ICP-OES

The X-Ray and ICP-OES Facilities are a full service and user facility. It features one powder X-ray diffractometer, one single crystal diffractometer, and one inductively coupled plasma optical emission spectrometer (ICP-OES) for use in research and teaching.

Electronics and Machine Shops

The support shops in the Department of Chemistry provide a variety of services to faculty, staff and students. Both are staffed with experienced professionals providing design, construction, and repair services to meet researcher needs.

Glassblower

Our professional glassblower, Eddie (Bo) Bishop, has over 35 years' experience in fabricating and repairing scientific glass. Bishop leverages his skills to create both traditional and custom items for UT researchers.

FOR MORE INFORMATION

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