FACULTY and RESEARCH in the
DEPARTMENT of CHEMISTRY
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Thank you for your interest in the research programs in the Department of Chemistry at the University of Tennessee's main campus, Knoxville.

We are proud of our long-standing tradition of excellence in chemical research and education. Our 30+ faculty members pursue research at the leading edges of modern chemistry, whether in the traditional divisional areas listed below or in exciting new interdisciplinary fields such as materials chemistry, environmental chemistry, and computational chemistry. We enjoy a close relationship with nearby Oak Ridge National Laboratory, a multiprogram Department of Energy research facility operated jointly by the University and Battelle Memorial Institute. Our students and faculty benefit from ready access to the laboratory's research facilities, which complement our already impressive in-house research instrumentation.

Our students and faculty have been recognized nationally and internationally for their research and teaching achievements. Several faculty members have received National Science Foundation CAREER awards, which are given to young faculty members who exhibit outstanding promise for future excellence in research and education. In recent years, three of our graduate students have won National Science Foundation predoctoral fellowships, and one of our students was among 60 graduate students from the U.S. chosen to attend the 56th anniversary annual meeting of Nobel Prize winners in Lindau, Germany.

This brochure describes the research programs of our individual faculty members. Each faculty member has a page on our departmental Web site (www.chem.utk.edu) that outlines his or her research in greater detail and lists several recent publications from her or his research group. We invite you to use this booklet and the Web site to learn more about our tradition of excellence in chemical research.

**Departmental Divisions**

**THE ANALYTICAL CHEMISTRY DIVISION** is composed of a dynamic group whose research spans most major areas of analytical chemistry including: mass spectrometry, separations, spectroscopy, sensors, and nanotechnology. Research in the analytical division is applied to solve problems in a number of scientific arenas such as process industrial chemistry, biology and environmental science. In addition to the core faculty in the analytical division, other chemistry faculty and adjunct faculty from Oak Ridge National Laboratory have research projects in analytical chemistry.

**THE INORGANIC CHEMISTRY DIVISION** at UT is a vibrant and dynamic group of faculty who undertake research in a surprisingly wide range of areas in the discipline. Ranging from fluorine chemistry to microelectronic and nanostructured materials, organometallic synthesis to lanthanide chemistry, almost virtually every branch of inorganic chemistry is represented in strength. Links to Oak Ridge National Laboratory provide an extra dimension, and several UT faculty conduct research at ORNL.

**THE ORGANIC DIVISION** pursues a rich diversity of modern research projects. Traditional synthesis programs involving natural products are complemented by extensive efforts to develop new synthetic pathways to therapeutic and diagnostic medicinal agents. An additional goal of the synthesis groups is the development and application of new methodologies, including environmentally friendly reaction procedures. All of these pursuits are supported by a complete suite of modern analytical and spectroscopic instrumentation useful in organic chemistry research.

**THE PHYSICAL CHEMISTRY DIVISION** conducts experimental and theoretical research in a wide range of areas: neutron and optical spectroscopic investigations of nanoscale, chemically active and magnetic materials; physical mechanisms for the production of chirality; x-ray and neutron spectroscopy of surfaces and materials; reaction dynamics and quantum chemistry; optical and electron spectroscopies; thermodynamics, computer simulation, and interfacial control of polymers; and film growth and surface chemistry. Many of our faculty are also involved in the synthesis and investigation of new materials.

**THE POLYMER CHEMISTRY DIVISION** at UT comprises a broad spectrum of activities ranging from the synthesis of novel polymer structures to the study of their physics and properties. Specific areas of interest include anionic polymerization; thermodynamics and properties of polymer solutions, blends, and nanocomposites; synthesis of linear and branched polymers and copolymers of controlled structure; polymer brushes; modification of polymer interfaces; Monte Carlo simulations; and the solid state of linear macromolecules. The neutron scattering and other facilities at Oak Ridge National Laboratory are extensively used.
Christopher A. Baker
Assistant Professor
Analytical Chemistry
B.S. Chemistry, Wayne State University (2006)
Ph.D. Analytical Chemistry, Florida State University (2012)
Postdoc, University of Arizona (2012-2014)
Postdoc, Sandia National Labs (2014)

We are developing new micro- and nanofluidic instrumentation, biomolecular assays, and biosensors to measure peptide-based cell-to-cell communications in and around the brain. Faster, higher sensitivity measurements will allow us to explore the roles of peptide signaling in behavior and may shed new light on mechanisms of neurodevelopmental disorders like autism.

David C. Baker
Professor
Organic Chemistry
Carbohydrate chemistry
Medicinal chemistry
B.S., University of Tennessee (1969)
Ph.D., Ohio State University (1973)
Editor, Carbohydrate Research

My group is involved in the design and synthesis of organic compounds that act as antivirals and as anticancer agents. We make use of computer modelling and knowledge of receptors and drug-receptor binding to aid in the design aspects. Compound types include carbohydrates and heterocyclic compounds, as well as nanostructures that are designed to mimic living cells.

Craig E. Barnes
Professor
Inorganic Chemistry
Organometallic chemistry
Transition metal-based catalysis
B.S., Harvey Mudd College (1977)
Ph.D., Stanford University (1982)
NATO Postdoctoral Fellow
Alexander von Humboldt Fellow

My research program focuses on developing new synthetic methodologies that target specific types of nanostructuring in heterogeneous catalysts. We are developing general procedures for preparing uniform dispersions single site catalysts that will be more active, more selective and more robust than traditional catalysts. Areas of application for these new heterogeneous catalysts are the conversion of biomass to fuels and fine chemicals, classic acid and oxidation catalysis and new olefin polymerization catalysts. Members of my group become well versed in three areas of science: synthetic chemistry, materials science and catalysis.

John Bartmess
Professor
Organic & Computational Chemistry
Gas phase ion chemistry
Mass spectrometry
Molecular orbital calculations
B.S., Rice University (1970)
Ph.D., Northwestern University (1975)

We are involved in separating the effects of intrinsic structure, solvation, and counter-ions on structure-reactivity relationships for organic reactions, via three areas of research. Solution calorimetry is being used to examine how “green solvents,” ionic liquids, interact with solutes. The chemical processes that occur in atmospheric pressure ionization sources for mass spectrometers, such as DART and APCI, is being determined. Computational chemistry is being used to both verify experimental energetics values, and to examine cases not experimentally accessible.

Michael D. Best
Associate Professor & Director of Graduate Studies
Organic Chemistry
Bio-organic, supramolecular and medicinal chemistry
B.S., Boston College (1997)
Ph.D., The University of Texas at Austin (2002)
NSF CAREER Awardee

Research in the Best Group utilizes bioorganic chemistry to understand biological processes involved in the onset of diseases such as cancer. Our primary focus involves chemical synthesis to obtain analogs of natural molecules for use as probes. We then employ the resulting compounds for biological studies aimed at understanding roles in physiological and pathophysiologic processes.

Tessa Calhoun
Assistant Professor
Analytical & Physical Chemistry
Chemistry & Life Sciences
Post-Doc, Lewis-Sigler Institute for Integrative Genomics, Princeton University
PhD, Chemistry from UC Berkeley
BS, Chemistry from Iowa State University

The Calhoun Lab investigates dynamical processes in biological systems through the development and implementation of ultrafast microscopy experiments. Current systems of interest include imaging the mechanisms of drug-membrane interactions in living yeast and bacterial cells. These measurements will provide new insight into the environmental factors responsible for the delivery and action of these drugs.
**Shawn Campagna**  
**Assistant Professor**  
Organic & Analytical Chemistry  
Chemical Biology, Metallo-peptide Catalysis, Metabolomics  
B.S., North Carolina State University (2000)  
Ph.D., Princeton University (2006)

Our lab integrates organic synthesis, bioanalysis, and biological tools to study the molecular level mechanisms of disease. We are currently focused on understanding infectious disease processes in bacteria and investigating metabolic diseases, such as obesity. We are synthesizing chemical probes to understand the mechanisms by which bacteria communicate during an infection and are also generating a number of natural product analogues to inhibit adipogenesis and fat accumulation.

We are actively synthesizing many chemical probes and developing new methods to interrogate biological phenomena. Our technique to detect and analyze a bacterial signal, DPD, implicated in the onset of infectious disease is shown above.

**Robert Compton**  
**Zeigler Professor**  
Physical Chemistry  
Negative Ion Chemistry, Fullerenes, Chirality  
B.S., Berea College (1960)  
M.S., University of Florida (1963)  
Ph.D., University of Tennessee (1965)  
AAAS Fellow APS Fellow OSA Fellow

My research involves experimental studies of singly- and multiply-charged negative ions including dipole (figure) and quadruple bound anions. We also perform fundamental studies in the area of chirality and have developed new methods for the study of linear and non-linear chiro-optical spectroscopy. A new area of research involves the storage of hydrogen in nanomaterials.

**Mark Dadmun**  
**Professor & UT/ORNL Joint Faculty**  
Polymer & Physical Chemistry  
Polymer blends and nanocomposites; neutron scattering studies of polymer interfaces  
B.S., University of Massachusetts (1967)  
Ph.D., University of Massachusetts (1991)  
NRC Postdoctoral Fellow NSF CAREER Awardee

Our research revolves around understanding how we can manipulate polymeric materials on a molecular level to allow the creation of polymer mixtures that will provide extraordinary properties, such as self-healing anti-microbial fibers and the next generation of solar cells. This is implemented by studying the thermodynamics and dynamics of polymer mixtures to provide the fundamental understanding necessary to guide the molecular level manipulation, implement the modification to the polymer molecules and testing the ultimate properties of the final mixture.

Figure depicting the dispersion of carbon nanotubes (black) in a matrix of polymer chains (blue). The aggregated morphology depicted in figure (a) is most likely from thermodynamics, but the dispersed mixture depicted in figure (b) is needed to attain much of the desired properties of polymer nanocomposites, such as their use in solar cells. We have recently developed methods to create dispersed systems using specific interactions between the polymer and nanotube.

**Sheng Dai**  
**Professor & UT/ORNL Joint Faculty**  
Inorganic & Analytical Chemistry  
B.S., Zhejiang University (1984)  
M.S., Zhejiang University (1986)  
Ph.D., University of Tennessee, Knoxville (1990)

The research projects of Dr. Sheng Dai focus on the synthesis and characterization of functional materials for energy-related applications. Currently, we are active in three fundamental investigations, each requiring the synthesis of functional materials for a targeted application. 1) Materials for Catalysis; 2) Materials for Separation; 3) Materials for Electrical Energy Storage.

**Ampofo Darko**  
**Assistant Professor**  
Synthetic Organic Chemistry  
Organometallic chemistry, organocatalysis  
B.S., Guilford College (2004)  
Ph.D., University of Florida (2010)

My research interests center on developing the scope of reactions involving strained molecules. Specifically, I am interested in the ability of strained molecules to accelerate reactions and influence their stereochemical outcomes. My group investigates this concept in the areas of organometallic catalyst design, cycloaddition reactions, and organocatalysis.

**Charles Feigerle**  
**Professor & Department Head**  
Physical & Materials Chemistry  
Raman spectroscopy  
Chemical vapor deposition  
Surface chemistry  
B.S., University of Illinois, Chicago (1977)  
Ph.D., University of Colorado (1983)  
NRC Postdoctoral Fellow

In my research group, we utilize Raman and other non-linear spectroscopies for analysis and characterization of fundamentally interesting molecules, materials, and physical processes. Recent projects include surface enhanced Raman analysis of an electrospray plume, studies of stress induced disorder-order transitions in polymers, and Raman aided structure determination of halogenated derivatives of C60. Raman analysis also has been instrumental in our development of diamond based stripper foils, foils used to convert H- to H+ in the beam line of the Spallation Neutron Source (SNS).

Left: A graphical model of the diamond based stripper foils used in the H- to H+ conversion.
Robert Hinde  
Professor  
Department of Chemistry  
Associate Dean  
College of Arts and Sciences  
Physical & Computational Chemistry  
Quantum chemistry; Reaction dynamics; Atomic and molecular interactions  
B.S., Rensselaer Polytechnic Institute (1987)  
Ph.D., University of Chicago (1992)  
NSF Postdoctoral Fellow  

We use ab initio quantum chemical computations and quantum Monte Carlo simulations to study the properties of low temperature, highly quantum condensed phases such as liquid He and solid H2. Through collaborations with experimental spectroscopists, we investigate the rovibrational dynamics of small molecules trapped in these low temperature liquids and solids. These studies provide detailed information on, and new insight into, intermolecular energy transfer phenomena in low temperature liquids and solids.  


David Jenkins  
Associate Professor  
Inorganic Chemistry  
Magnetic materials, organometallic chemistry, catalysis.  
Ph.D., California Institute of Technology (2005)  
NSF Graduate Fellow; Miller Institute for Basic Research in Science Postdoctoral Fellow  

My research focuses on synthesis to produce novel chemical systems to investigate two distinct areas of inorganic chemistry, organometallic catalysis and magnetic materials. For the organometallic catalysis project, we are developing tetracarbene macrocycles for use in group transfer reactions and small molecule activation. For the magnetic materials project, we are synthesizing metal organic frameworks that undergo spin crossover for a variety of applications including gas separation and storage.  

Tetracarbene ligands for organometallic catalysis projects.

George Kabalka  
Alumni Distinguished Service & Cole Professor  
Organic & Medicinal Chemistry  
Organoboron chemistry; positron emission tomography; magnetic resonance imaging  
B.S., University of Michigan (1965)  
Ph.D., Purdue University (1970)  
AAAS Fellow  

A primary goal of Dr. Kabalka’s research centers on the design and synthesis of pharmaceuticals labeled with radioisotopes for use in the Positron Emission Tomographic (PET) evaluation of neurodegenerative diseases, such as Alzheimer’s and Parkinson’s, as well as neurological disorders involving seizure activity and tumor growth. The detection of cancers, such as metastatic malignant melanomas and glioblastomas, is also an important component of the research program.  

Positron Emission Tomographic (PET) Scans of Post-Therapy Patient Using 18F-BPA-Fructose (left) and 11C-ACBC (right) – Reagents created at the University of Tennessee by members of the Kabalka group.

S. Michael Kilbey II  
Professor & UT/ORNL Joint Faculty  
Polymer Chemistry  
Structure and properties of ultrathin polymer films at surfaces  
Molecular assemblies in solution  
B.S., University of Wisconsin (1990)  
Ph.D., University of Minnesota (1996)  

Our research activities focus on the self-assembly, structure, and interactions of polymers at interfaces, including architecturally complex block copolymers and bio-inspired polymers. Through a variety of molecular-level measurements, we aim to understand how manipulating the size, arrangement, and type of building block alters structure and properties. Because materials communicate with their environment via their interfaces, these fundamental studies provide guidance for the design of systems with improved interfacial properties that find application in biotechnology, separations, or diagnostics.  

Figure. Self-assembled polymer micelles.

Jeffery Kovac  
Professor & Director of Undergraduate Studies  
Physical & Polymer Chemistry  
Statistical mechanics; history and philosophy of science; scholarship of teaching and learning  
B.A., Reed College (1970)  
Ph.D., Yale University (1974)  
AAAS Fellow  

My interests are in statistical mechanics and thermodynamics of condensed matter, primarily polymer systems. We have used both computer simulation methods and analytical theory to study a wide variety of systems ranging from simple models of polymers and fluids to a complex natural material -- bituminous coal.  

Autocorrelation function for the relaxation of the normal modes of a polymer adsorbed on a solid surface.
We combine materials chemistry, thermodynamics, neutron scattering, and computer modeling to study the structure and dynamics of novel materials. Our focus is on the behavior of molecules adsorbed into surfaces or entrained within porous media. We strive to develop materials with unique chemical/physical properties that can be used as sensors, catalysts, gas/energy storage devices, and in optoelectronics. We have international neutron scattering activities that include the development of VISION, a “best in class” next generation neutron vibrational spectrometer for the Spallation Neutron Source.

Neutron diffraction line shapes for a 2D commensurate (c2x2) (a) and hexagonal compressed monolayer (b) solids of H2 adsorbed on a MgO(100) surface. Cartoons of these 2D structures illustrating the oblate rotational motion of the H2 films appears in (c) and (d), respectively. This is representative of our work in H2 interactions with nanomaterials. See J.Z. Larese et al., Phys. Rev Letters (2008).

Figure: Dissociation of single oxygen molecules on a silver surface using the scanning tunneling microscope.

Research in the Long group focuses on the synthesis and application of functional macromolecules and catalyst design. We utilize the tools of organic synthesis, polymer chemistry, and organometallic design in an interdisciplinary approach to address academic problems with real world impact. Our research has three themes: (1) the design, synthesis, and application of conducting organic polymers, (2) the development of organometallic polymerization catalysts, and (3) recyclable catalysts for stereoselective control.

Research in the Musfeldt group focuses on the spectroscopic response of low-dimensional, molecular, and nanoscale solids, with the goal of understanding the consequences of microscopic strain, high magnetic fields, and chemical substitution on the local structure and functionality. Recent initiatives include charge and bonding problems in nanoscale transition metal dichalcogenides, magnetic field-induced optical contrast in spin ladder materials, spectroscopic investigations of charge ordering, magnetoelastic coupling, structure–property relations in multiferroics, and band gap tuning of oxide heterostructures for solar energy applications.

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We combine materials chemistry, thermodynamics, neutron scattering, and computer modeling to study the structure and dynamics of novel materials. Our focus is on the behavior of molecules adsorbed into surfaces or entrained within porous media. We strive to develop materials with unique chemical/physical properties that can be used as sensors, catalysts, gas/energy storage devices, and in optoelectronics. We have international neutron scattering activities that include the development of VISION, a “best in class” next generation neutron vibrational spectrometer for the Spallation Neutron Source.

Neutron diffraction line shapes for a 2D commensurate (c2x2) (a) and hexagonal compressed monolayer (b) solids of H2 adsorbed on a MgO(100) surface. Cartoons of these 2D structures illustrating the oblate rotational motion of the H2 films appears in (c) and (d), respectively. This is representative of our work in H2 interactions with nanomaterials. See J.Z. Larese et al., Phys. Rev Letters (2008).

Figure: Dissociation of single oxygen molecules on a silver surface using the scanning tunneling microscope.

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**Michael Sepaniak**  
**Zeigler Professor**  
Analytical Chemistry  
Capillary separations; chemical sensing;  
Laser spectroscopy  
B.S., Northern Illinois University (1974)  
Ph.D., Iowa State University (1980)  
AAAS Fellow

In recent years, we have capitalized on advances in materials science and micro- and nano-fabrication technology to enhance chemical analysis in the traditional “three Ss:” Separations, Spectroscopy (optical), and Sensing. Specifically, we use advanced lithographic techniques and nanostructuring strategies to produce silicon pillar systems and microcantilever surfaces that are further modified chemically. These systems are then used for chemical separations, surface enhanced Raman spectroscopy, and nanomechanical-based sensing, all with enhanced analytical figures of merit.

Enantio-selective sensing using antibody-mediated nano-mechanical bending of functionalized cantilevers

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**Bhavya Sharma**  
**Assistant Professor**  
Analytical Chemistry  
Postdoctoral Research, Dept. of Chemistry, Northwestern University  
Ph.D. in Chemistry, University of Pittsburgh

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 to interrogate biology. Specifically, we are developing methods for early detection of disease (both in vitro and in vivo detection), as well as methods for chemical and biological sensing.

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**Alexei Sokolov**  
**Governor’s Chair, Professor**  
Department of Chemistry and Department of Physics & Astronomy  
M.S. in Physics, Novosibirsk State University, Russia (1981)  
Ph.D in Physics, Academy of Sciences of USSR (1986)  
Habilitation (Dr.Sci.), Russian Academy of Sciences

Our research interests are focused on the dynamics and mechanical and optical properties of soft materials, ranging from polymers to nano-composite and nano-structured materials, to biological systems. We are developing molecular level understanding of physical and chemical processes that control macroscopic properties of soft materials. This knowledge provides a key to design new materials for various energy and bio-tech applications.

Illustration of materials studied in our group

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**Frank Vogt**  
**Associate Professor & Associate Head**  
Analytical Chemistry  
Optical sensors; chemometrics;  
Chemical imaging  
2007 ORAU Ralph Powe Faculty Enhancement Award

Analyses of heterogeneous samples require innovative chemical sensors that determine spatial distributions of analytes. We develop new sensors by combining optical spectroscopy with modern imaging techniques (‘spectroscopic imaging’). Our analytical concepts facilitate fast chemical sensing at high resolution in two and three spatial dimensions.

The figure shows an example: spectroscopic imaging enables material classification over long distances.

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**Ziling (Ben) Xue**  
**Ziegler Professor**  
Inorganic and Analytical Chemistry  
Synthetic and mechanistic organometallic/inorganic chemistry;  
Molecular approaches to advanced materials;  
Sensor and new chemical analysis.  
B.S., Nanjing University of Pharmacy - Nanjing University (1982)  
Ph.D., University of California, Los Angeles (1989)

Our research program is centered on two areas: (1) organometallic-inorganic chemistry related to the formation of microelectronic materials, and (2) new analytical methods. These areas involve research in both fundamental chemistry and applications in high-tech materials. The research gives us opportunities to practice the science of molecular and solid-state synthesis and to understand the fundamental mechanistic pathways in the reactions.


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**Bin Zhao**  
**Professor**  
Polymer Chemistry  
Environmentally responsive polymers and polymer brushes; “living”/controlled polymerization; polymer surface chemistry  
B.S., University of Science and Technology of China (1992)  
M.S., University of Science and Technology of China (1995)  
Ph.D., University of Akron (2000)

My research interests center on environmentally responsive polymeric systems, including thermosensitive water-soluble polymers, well-defined homopolymer brushes, and responsive polymer brush-grafted particles. “Living”/controlled polymerization techniques are being used to synthesize polymers and polymer brushes with controlled molecular weights, narrow polydispersities, and defined architectures. These soft materials have potential applications in controlled encapsulation and triggered release of substances, surface-responsive materials, smart catalysis, biotechnology, and nanotechnology.

Schematic illustration of multiple micellization and dissociation transitions of a thermo- and light-sensitive block copolymer in water.