# Truman State University CHEMISTRY Faculty Research Interests

**Dawood Afzal** (Organic): Dr. Afzal's research interests are in several areas covering a wide range of topics. These include:

1. Macrocyclic chemistry especially chemistry of porphyrins and metalloporphyrins. This research focuses on the syntheses, structure and study of reaction chemistry of the previously mentioned molecules.
2. Synthesis of layered compounds, especially metal oxide perovskites using high temperature solid state reaction. These perovskites have potential application as catalysts, semiconductors, magneto-resistive substances.
3. Nuclear Magnetic Resonance (NMR) spectroscopic study of compounds to understand their chemical structure and also to monitor chemical reactions.
4. Transition metal organometallic chemistry. In this area the focus is on developing new synthetic methodology and exploring new chemistry of transition metal compounds as well as their application in organic syntheses.

Students have a wonderful opportunity to have hands on experience with a wide range of synthetic techniques and equipment. Dr. Afzal's research lab has a wide range of dedicated equipment for specialized chemical synthesis Such as an inert atmosphere glove box for manipulation of air and moisture sensitive compounds under dry nitrogen atmosphere, Schelenk lines and high vacuum lines, High temperature furnaces and Sonochemical equipment for carrying reactions with ultrasound. In addition, Dr Afzal's group routinely uses spectroscopic techniques such a Uv-vis , IR and NMR and X-ray diffraction analysis.

**Russell Baughman** (Physical/Crystallography): Dr. Baughman and his students determine the 3-D structures of molecules using X-ray Crystallographic (lab & computer work) and Quantum Mechanical (theoretical/computational) methods. Their objective is to gain better insight into how a molecule's structure affects its ability to react. To do this they investigate the molecule's geometry/shape at a high level of precision (usually 4 significant figures for bond distances and angles) and thereby gain an understanding about the manner in which the molecule's bonding occurs.

The main lab tool used is an X-ray diffractometer) with which crystalline materials can be analyzed. Specifically, they can often take a "small" crystal (0.3-0.5 mm on an edge!) and obtain the precision that is necessary to gain the insight mentioned above. Dr. Baughman and his students have worked on and published articles in professional journals on the structure-activity relationships of small biologically active molecules (pesticides, drugs, etc.) and "charge-transfer" complexes which conduct electricity in one direction and insulate in the other two directions. In addition, they collaborate with a number of the Truman State chemistry faculty to resolve their questions (and end up learning a lot of other interesting chemistry!).

**Kenneth Carter, Jr.** (Physical): Dr. Carter has interests in chemometrics and other applications of statistics, mathematics, nonlinear dynamics, and computational modeling to chemistry or the environment. His recent research focus has been the calculation of confidence limits, which are indicators of the trustworthiness of quantitative results. Ongoing work of confidence limits, which began with data analysis for a particular general chemistry lab, has so far resulted in a student co-authored paper in the world's most widely circulated peer-reviewed journal of analytical chemistry, and in several presentations by students at meetings of the Missouri Academy of Science. Dr. Carter has also worked with students and presented papers in the interdisciplinary field of the relationship of science and religion.

**Dana Delaware** (Organic/Biochemistry): Dr. Delaware's broad research interest is in the area of medicinal chemistry that involves the development and investigation of new or better pharmaceutical agents. A long-term project involves the modification of the monosaccharide fructose as a potential anti-tumor agent. New projects are investigating the development of new bioanalytical techniques involving Capillary Electrophoresis. Presently, his research community is analyzing vitamins from different food sources and benzodiazepines by Capillary Electrophoresis. Educational pedagogy in the teaching of organic chemistry and biochemistry continues to be a research interest in collaboration with other Chemistry faculty at Truman.

Students have presented papers and posters at Truman Undergraduate Research Symposium, Missouri Academy of Science, Midwest Regional American Chemical Society meetings, and National Conference of Undergraduate Research .

**Roger Festa** (Chemical Education): Dr. Roger Festa studies both the process and outcomes of undergraduate professional training in chemistry. He continues his series of papers applying student development theory to the professional development of college chemistry majors, focusing on the applications of the American Institute of Chemists Code of Ethics to professional conduct. A collateral interest is the development of a model application of student development theory and a holistic approach to professional advising. Dr. Festa also studies and serves as a consultant to undergraduate chemistry departments at liberal arts colleges, particularly those departments that are "at risk" and have deviated from the culture of American academic chemistry.

**Victor Hoffman** (Organic): Dr. Hoffman has ongoing research interests in synthesizing ATP antagonists. These ANAPP3 derivatives are synthesized by using different amino acids (glycine, alanines, and aminobutric acids) to link an arylazido group to ATP molecules. The research has expanded to synthesize other ATP type antagonists that target a specific P2 receptor site.

**Barbara Kramer** (Analytical): Dr. Kramer's research interests lie in following the fate of various pollutants in the environment. Currently, her group is examining the fate of pesticides applied to the soil. These compounds include classes of chemicals that have been shown to be toxic to humans and animals. When soil samples are analyzed for the presence of organic contaminants, they are subjected to harsh extraction conditions in order to find all of the compound that is present in the soil system. These extractions, while giving useful information about the total contamination level, do not help identify the risks of exposure to the chemical when someone is actually exposed to these soils. When soil is consumed (accidentally or intentionally) not all of the contaminants present in the soil will be released and able to cause a physiological response. The portion that is released into systemic circulation is considered bioavailable. The amount of a given compound that is bioavailable will depend on the compound, the soil type and how long the compound has been present in the soil, among other things.

Traditional exposure assessment tests typically involve animal models or complex models of the human digestive system. One of the goals of her research is the development of a simple analytical method that can be used to model bioavailability. Her group is currently investigating the optimization of an aqueous microwave assisted extraction technique to model a more complex bioavailability method involving a model of the human digestive system.

In order to understand the aspects of an overall soil system that contribute to the bioavailability of a compound, Dr. Kramer's group is also investigating methods of understanding the physical and chemical interactions between organic contaminants and the soil. Current methods under investigation include sequential extractions using increasingly more severe methods in order to study the ease by which different compounds are removed from the soil.

As bioavailability will depend on the type of soil that is contaminated, several different types of soil with varying amounts and types of inorganic and organic components are being studied. In order to isolate the components of the soil that contribute to the retention of specific compounds, Dr. Kramer's group isinvestigating the development of an artificial soil whose composition can be controlled.

**Brian Lamp** (Analytical): Dr. Lamp's research interests are in the areas of surface design and electroanalytical chemistry. Electroanalytical techniques are based on the oxidation and reduction of species in solution and hold promise in the sensor arena because they are relatively straightforward, robust, and cost-effective. Many of the challenges in electrochemical measurements center on the ability of the technique to distinguish one analyte from another. Most of Dr. Lamp's projects are aimed at improving this "selectivity" for electroanalytical measurements.

Specifically, Dr Lamp is interested in the design and character-ization of modified electrode materials with locally tunable chemical and electrochemical activity. In these projects, students working with Dr. Lamp attempt to "build in" some selectivity by controlling the chemistry that occurs on portions of the sensor surface. Such surfaces will be useful in enhancing the selectivity of electrochemical devices and will have importance in the design of miniaturized sensors.

In order to construct and characterize these surfaces, it is critical to be able to study their local reactivity with fairly high spatial resolution. As a result, Dr. Lamp is also very interested in the development of techniques that allow spatial and chemical characterization of such interfaces. To address some of these concerns, Dr. Lamp and his students have constructed a scanning electrochemical microscope, capable of "mapping" the activity of a surface at micrometer ($10^{-6}$m) resolution.

**James McCormick** (Physical Inorganic): Dr. McCormick's research is very cross-disciplinary involving aspects of inorganic, organic, analytical and physical chemistry. While it is primarily directed toward understanding the chemical reactions of metal ion coordination complexes (physical inorganic, analytical) there is a major synthesis component (organic, inorganic). Depending on a student's interest, he or she could pursue research that is purely synthetic, purely physical or some combination of the two.

Two projects are currently available. One explores the role of the lone pair of electrons in the chemical reactions of main-group metal ion coordination complexes. VSEPR theory predicts that a lone-pair in main-group metal complexes occupies a site in the coordination sphere about the metal (said to be stereochemically active), but recent work has shown this is not always the case. The questions that need to be answered are: what leads the lone pair to be stereochemically active? can this be quantified? and does the stereochemical activity of the lone pair affect the chemical reactions that these complexes undergo? The implications of this work are far-reaching, ranging from a deeper understanding of the toxicity of these metals *in vivo* to explaining the properties of semiconductors that incorporate main-group metal ions. The second project is investigating the reactions of ozone ($O_3$) with transition metal coordination complexes. The activation of oxygen by transition metal complexes for reaction with organic molecules is of fundamental importance in biochemistry and to industry. This process is, however, poorly understood. To gain insight into these reactions, $O_3$ will be used to directly generate and study the intermediates believed to be important in the oxygen chemistry. Since $O_3$ is a more powerful oxidant than $O_2$ it is an attractive means to efficiently destroy toxic substances at moderate temperatures and pressures, additional effort will be directed toward the development of transition metal complex catalysts for these processes.

**David McCurdy** (Analytical): Dr. McCurdy's research interests are in the area of analytical chemistry. His current work includes: (1) the Development of Methods for Trace-Level Elemental Analysis using Atomic Spectroscopy (including the Inductively Coupled Plasma, Direct Current Plasma, and Flame and Furnace Atomic Absorption Spectrophotometry), (2) the Development and Applications of Methods of Sample Introduction in Plasma Emission Spectrometry, (3) the Preparation and Treatment of Samples for Analysis, (4) the Development of New Laboratory Experiences for Undergraduate Classes in Analytical Chemistry, and (5) the Advancement of Undergraduate Research.

Modern methods for the analysis of trace ($10^{-3}$ to $10^{-6}$ %) and ultra-trace ($10^{-6}$ to $10^{-9}$%) level elements rely heavily on the use of atomic spectroscopy, particularly the use of the inductively coupled plasma (ICP), direct current plasma (DCP), and graphite furnace atomic absorption spectrophotometry (GFAAS). In particular, the ICP and DCP have gained wide acceptance as the "instrument of choice" by analytical chemists because of their speed, sensitivity, selectivity, and simultaneous multielement capabilities.

Despite the power of plasma methods, they are not free from weakness. The introduction of samples into the ICP or DCP is considered to be a weak link in plasma spectroscopy. Much of Dr. McCurdy's research work is aimed at developing new approaches for the introduction of solid or microliter/microgram-quantity samples into the ICP and DCP. The work includes projects which are designed to reduce the amount of time and effort in preparing samples for rapid ICP and DCP elemental determinations, to develop methods for the direct introduction of solid samples, and to investigate methods of introduction of microsamples.

Other projects being pursued in Dr. McCurdy's lab include methods of sample preparation for analytical chemistry using microwaves and the development of other forms of sample introduction for plasma spectroscopy, including slurry nebulization and thermospray nebuilzaiton, as well as means for increasing detection capability in atomic spectroscopy.

**Anne Moody** (Organic): Physical Organic Chemistry; Natural products of plants and mushrooms, Organic Chemistry education in both classroom the laboratory settings.

Plant and fungal organic natural products can be isolated from locally collected materials, structurally characterized by spectroscopic and chemical means, and examined for bioactivity. The choice of the sources of the natural products is driven by folklore reports of medicinal use of these plants and mushrooms. For example, quinones are ubiquitous in nature, serving a variety of functions in plants and animals. Dr. Moody is also investigating the photochemical dimerization of quinones reportedly found in various impatiens plants.

**Maria Nagan** (Computational Biochemistry): Dr. Nagan's group is interested in understanding ribonucleic acid (RNA) recognition by computationally modeling protein-RNA and RNA-RNA interactions. The primary computational method used is molecular dynamics, which is based upon a classical model that allows the simulation of a molecule's motions throughout time. Dr. Nagan is interested in modeling RNA because it can form unusual structures in addition to standard double helices.

Organisms called "extremophiles" tend to live in high salt concentrations, at high pressures, in anaerobic environments or in extreme temperatures. In addition, these extremophiles possess unusually high amounts of posttranslationally modified nucleic acid bases in their transfer RNA. Dr. Nagan is interested in understanding why modified bases are required in transfer RNA molecules and specifically the chemical role that they play. Students in Dr. Nagan's group are also interested in understanding protein-RNA recognition at various points in the life cycle of the HIV-1 virus. Blocking protein-RNA binding can inhibit the ability of HIV to replicate. Thus, understanding how and why proteins recognize specific RNA molecules in HIV may lead to future antiviral agents.

**John O'Brien** (Inorganic/Supramolecular): Dr. O'Brien's group is oriented towards synthetic chemistry, currently has several projects utilizing transition metals in organic synthesis, either as catalysts or as reaction templates, to make large rings of atoms, or macrocycles. Additionally, his group studies the macrocyclic products of our synthetic efforts as models for living systems. Examples of how living systems use transition metals include photosynthesis in plants (chlorophyll) and oxygen transport in animals (hemoglobin). Interestingly, the active sites of both hemoglobin and chlorophyll incorporate the same naturally occurring macrocycle, porphyrin. Dr. O'Brien's macrocyclic research focuses primarily on oxygen carriers and involves the synthesis of new macrocyclic ligands (not porphyrins) which, when furnished with the proper transition metal, can act as reversible oxygen carriers and thereby model the performance of hemoglobin.

Dr. O'Brien's group is also interested in modeling the protein portion of globular proteins. In his group, this is accomplished by forcing extremely large rings (30-40 atoms) into interesting shapes such as threaded or interlocked rings (rotoxanes and catenanes, respectively) and knots. The concepts of this project, which is supramolecular in nature, are relatively easy to understand, but are rather difficult to put into practice.

**Eric Patterson** (Computational Organic): Dr. Patterson's research group is interested in understanding the fundamental properties and reactivities of a wide variety of organic molecules. His students employ a method generally known as *ab initio* (Latin: from first principles) molecular orbital theory. This method is based upon quantum chemistry, and allows the accurate prediction of molecular shapes, energies and properties. His group applies these methods to study a number of interesting systems, including:

- The neutralization and destruction of the chemical warfare agents such as VX and sarin.
- The fate and remediation processes of chlorinated organic wastes which contaminate our drinking water.
- The properties and reactions of highly unstable molecules known as carbenes and carbynes.
- The properties and reactions of organometallic species (molecules which are largely organic in nature, but contain one or more metal atoms).

**Vaughan Pultz** (Physical): Vibrational Circular Dichroism; Leaching of Barium and Copper from ceramic glazes

**Peter Ramberg** (History of Science): Dr. Ramberg is the resident historian of science in the Division of Science and also teaches organic chemistry. His specialty is the history of nineteenth century chemistry in Germany, and he recently completed a book manuscript on the early history of stereochemistry from the proposal of the tetrahedral carbon atom in 1874 by J.H. van 't Hoff and J. A. Le Bel to the isolation of the first optically active inorganic compound by Alfred Werner in 1914.

Dr. Ramberg is interested generally in understanding chemistry as a discipline and its development since the seventeenth century, and his research has been guided by the goal of providing historical answers to philosophical questions in chemistry, including the meaning of chemical formulas, the foundations of atomism in chemical theory, the relationship between chemical theory and experiment, chemistry's relationship to physics and biology, and reductionism and mechanism in chemical theory. He is also interested in the role that recreation of historic experiments in chemistry and other sciences can play in our understanding of the scientific process.

**David Wohlers** (Inorganic): Dr. Wohlers is interested in studying the synthesis of acyl and alkylmetalloporphyrin complexes to investigate potential catalytic application in carbonylation and polymerization reactions. He is involved in the investigation and discovery of enhancements for the visually impaired in science education. He is also interested in the synthesis of compounds containing seven or more elements (for the fun of it!).