

Faculty Research Interests

Chemistry Department, USNA

Faculty members at USNA are not only engaged in the traditional teaching/learning processes typically associated with undergraduate institutions, but they are also a world-class faculty in terms of involvement in research. Midshipmen have many opportunities to participate in research or capstone project courses, especially during the 1st class year. Below are listed brief summaries of the research interests of the current Chemistry Department faculty at USNA. More detailed summaries for the faculty are found at the Chemistry Department website: <http://www.usna.edu> (and follow the links).

Analytical Chemistry

Prof. Graham T. Cheek. The electrochemistry of organic compounds, including mechanistic studies and preparative aspects. Use of room-temperature molten salts (or ionic liquids) as solvents. These systems are very attractive for use in "green chemistry" (environmentally friendly) applications because they have very low vapor pressures.

Prof. Christine L. Copper. Development of separation and detection methods for important molecules. Specifically, capillary electrophoresis methods are being developed to study environmental pollutants and chemical/biological warfare agents. These projects are performed in conjunction with researchers at the Naval Research Laboratory.

Assoc. Prof. JudithAnn R. Hartman. Solid, solution, and gas phase structural studies of transition metal complexes containing novel tripodal ligands. Sol gel synthesis and study of functionalized silica gels designed to remove metal ions from jet fuels or wastewater.

Asst. Prof. Dianne J. Luning Prak. Overall research focuses on the use of chemical surfactants to enhance the solubility and chemical or biological degradability of organic compounds. Recent efforts have focused on the solubility of nitroaromatic compounds in seawater and surfactant solutions. Future work will examine the degradation rates of energetic compounds such as TNT.

Assoc. Prof. Daniel W. O'Sullivan. Development of novel analytical methods and design of innovative sampling systems for the analysis of compounds in marine and atmospheric systems at ambient levels. Utilize the analytical techniques to evaluate the impact that chemical speciation, photochemistry, and redox reactions have on the transport, distribution, and biogeochemistry of different chemical compounds in the environment.

Assoc. Prof. Maria J. Schroeder. Characterization and applications of specialized polymeric systems (elastomers, networks, gels, and coatings). Research collaboration with the Naval Research Laboratory and US Army. Current projects include designing new polycarbonates for transparent armor applications, testing polymer coatings for blast protection on Humvees, and using polymers to reduce drag on small Navy vessels.

Asst. Prof. Ronald L. Siefert. Dr. Siefert's research interests include atmospheric and aquatic chemistry. Dr. Siefert is interested in the chemical processing of atmospheric aerosols and their role as a source of chemical species (e.g., nutrients) to remote and coastal surface waters. Understanding these atmospheric sources is important since they can control ecological processes.

Assoc. Prof. Paul C. Trulove. Development of nanoscale composites of polymers and bio-polymers with layered silicates and/or carbon nanotubes. Characterization of the physical, chemical, optical and electronic properties of these novel materials for potential applications in areas such as ballistic protection and low-observables (stealth). Work performed in collaboration with the Air Force Research Laboratory and the National Institute for Standards and Technology. Development of new ionic liquids for applications in high-energy density batteries. Characterization of the physical, electrochemical, and thermal properties of the ionic liquids. Work performed in collaboration with the Naval Research Laboratory.

Biochemistry

Asst. Prof. Daniel P. Morse. RNA (ribonucleic acid) performs a remarkable variety of functions in cells. It is best known for its role in protein synthesis: mRNA is the template that codes for protein; tRNA carries amino acids to the site of protein synthesis; rRNA is the major component of ribosomes which are the molecular machines that carry out protein synthesis. In recent years many other types of RNAs have been discovered that carry out surprising new

functions. I am interested in RNA function and how a process called "RNA editing" can alter the function of an RNA molecule by changing its sequence. I have identified many new RNAs that undergo RNA editing. I am currently trying to understand the biological consequences of these editing events and I am developing new methods to detect edited RNAs.

Asst. Prof. Brian Rehill. My research focuses on ecology, especially the chemical mediation of animal-plant interactions. For example, I collaborate on a project that investigates the relative roles of plant genetics and chemistry on community and ecosystem processes, using hybrid cottonwood trees and their associated fauna. Other projects study plant chemical effects on herbivore physiology, possible effects of climate change on plant-animal interactions, and the variability of plant chemistry in nature. As part of this work, student projects can include significant amounts of natural products and analytical chemistry.

Asst. Prof. Jamie L. Schlessman. Protein structure-function studies, using x-ray crystallographic and biochemical methods, are my research focus. I am determining the crystal structures of a series of mutants of Staphylococcal nuclease to probe the effects of inserting ionizable residues into the protein interior. Another project involves the isolation of proteins from psychrophilic bacteria, which live at near-freezing temperatures. These proteins will be studied to identify potential molecular adaptations to cold environments.

Asst. Prof. Virginia F. Smith. A variety of biophysical and biochemical methods are used to understand two biological problems: 1) the method by which methionine sulfoxide reductase A (MsrA) recognizes oxidatively damaged proteins and 2) the properties of the bifunctional protein cytoplasmic aconitase/iron-regulatory protein-1, which plays a key role in iron regulation in mammals.

Computational Chemistry

Prof. Mark L. Elert. Computer simulation of shock waves and detonation in condensed-phase materials. Molecular dynamics simulations are used to predict reaction products, detonation velocities, and shock wave structures.

Prof. Judith A. Harrison. Computational modeling of friction, wear, and adhesion in hydrocarbon systems. In particular, we hope to use our atomistic results to explain phenomena measured with Scanning Probe Microscopes.

Assoc. Prof. Joseph J. Urban. Computational Organic Chemistry. The structure-activity relationships and conformational properties of organic compounds, primarily those with biological activity, are studied using computer modeling techniques.

Chemistry Education Research

Asst. Prof. Clare E. Gutteridge. We are developing a laboratory sequence to illustrate to midshipmen how a drug program operates. An assay to measure antibacterial activity of organic molecules has been developed, which will be used to test molecules synthesized by midshipmen. In the future we intend developing experiments to introduce of the modern synthetic method of combinatorial chemistry (which allows many molecules to be made simultaneously) to the teaching laboratory.

Asst. Prof. Shirley Lin. Development of IL2/IL4 experiment on multistep synthesis. The project will involve some literature searching, laboratory synthesis and characterization of organic and organometallic compounds.

Assoc. Prof. Maria J. Schroeder. Development of new laboratory experiments for the integrated laboratory courses with particular focus on those involving military applications and analytical instrumentation, although any areas of student interest will be considered. Development of new laboratory experiments for a Chemistry of Cooking special topics class.

Inorganic Chemistry

Assoc. Prof. William B. Heuer. Synthesis and Characterization of electronically-delocalized transition metal complexes and organic dyes exhibiting novel electronic, magnetic and/or optical properties. Studies of supramolecular ("host-guest") complexation of these molecules related to development of materials for non-linear optical, electroluminescent and photovoltaic applications.

Assoc. Prof. Joseph F. Lomax. Synthesis and characterization of new metal phosphates, with potential applications in fuel cells. Creation of new inorganic laboratory experiments such as one on intercalation chemistry.

Asst. Prof. Amy Roy MacArthur. Research interests lie in the design, synthesis, and application of transition-metal complexes as catalysts for organic reactions. This work involves both organic and inorganic synthesis, along with characterization methods such as NMR, GC, and UV-vis spectroscopy, as well as X-ray crystallography. Elucidation of reaction mechanisms via detailed kinetic studies will also be pursued.

Assoc. Prof. Wayne H. Pearson. Structure determination using single crystal X-ray diffraction. Current areas of interest include high pressure crystallography of explosives in diamond anvil cells, crystal engineering of mineral systems and electron density determination in small molecules using multipole refinement techniques.

Prof. J. E. Shade. Synthesis and characterization of stereoisomers of transition metal complexes under thermal and photochemical conditions. The identity of the ligands and solvent, reaction temperature and wavelength of the photolysis lamp are investigated as variables which affect the identity and ratio of the products. Reaction progress and product characterization includes multi-nuclear and multi-dimensional NMR, IR and X-ray diffraction.

Organic Chemistry

Assoc. Prof. Debra Dillner. Research is being carried out in the general area of synthetic organic chemistry and NMR spectroscopy. In synthesis, several projects are ongoing. One is preparation of a series of nucleoside analogs. These compounds should have interesting biological activity and once prepared will be tested for antiviral properties. Another project is preparation of simple derivatives of menthol, a terpene. Once the compounds are prepared, their NMR spectra are obtained and interpreted.

Prof. Jeffrey P. Fitzgerald. Current research is directed towards the design and synthesis of novel materials. One project is to create molecules capable of catalyzing low temperature reactions of oxygen. A second project is to create optical limiters – nonlinear optical materials which are transparent to ambient light but opaque to laser light.

Asst. Prof. Clare E. Gutteridge. Malaria is a threat to the warfighter and civilian alike, globally causing a death every 30 seconds. Using known and novel organic reactions to prepare easily-synthesized molecules with potential as antimalarials, we aim to develop an antimalarial drug candidate in collaboration with the US Army.

Assoc. Prof. Chris M. Kinter. Synthesis of organic compounds for the study of neuroreceptors. Synthesis of radioactively labeled compounds for use in neuroreceptor imaging by PET (positron emission tomography) and SPECT (single photon emission tomography).

Asst. Prof. Shirley Lin. Catalysis, Self-Assembly and Molecular Recognition. Three available projects: 1) Development of novel synthetic routes to polymers and block copolymers. 2) Synthesis and self-assembly of block copolymers through noncovalent interactions. 3) Study of small-molecule additives to facilitate protein crystallization (in collaboration with Asst. Prof. Jamie Schlessman).

Assoc. Prof. Craig M. Whitaker. The main objective of my research is to develop novel, functionalized single-walled carbon nanotubes (SWNTs) for energetic materials in collaboration with NWSC Indian Head Laboratory. The functionalized carbon nanotubes will be incorporated or bound into propellant matrices for different energetic applications. The goal is to significantly enhance the initiation, overall propellant performance, safety, as well as the mechanical properties.

Physical Chemistry

Prof. Mark L. Campbell. Gas phase kinetics of oxidation reactions of lanthanide and transition metal atoms. Two laser experiments are performed where one laser photolyzes a precursor molecule and laser induced fluorescence is used to monitor the temporal profile of the metal atom. Rate constants as a function of temperature and pressure are determined and used to calculate activation energies and reaction mechanisms.

Prof. Robert F. Ferrante. Low temperature (~10 K) spectroscopy of stable and unstable molecules. Particular interest is focused on modeling the compositions and reactions of ices in comets and other astrophysical objects, by the spectroscopic study of analogous laboratory samples, in collaboration with astrochemists at the NASA/Goddard Space Flight Center.

Assoc. Prof. Roy E. McClean. Gas phase kinetic studies of transition metal atoms with sulfur dioxide using a laser photolysis / laser-induced fluorescence technique. Computational studies on the binding energies and structural parameters of transition metal – sulfur dioxide isomers are also performed.