

# **The A.R. Smith Department of Chemistry**

## **Overview of Faculty Research Interests**

**Spring 2016**

### **Dr. Carol Babyak**

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Dr. Babyak teaches Introductory, Analytical, and Environmental Chemistry classes at Appalachian State University. She holds a Ph.D. in Analytical Chemistry from West Virginia University (WVU) under the guidance of Dr. Ronald B. Smart. Her research involved the development of electrochemical methods for the detection mercury emitted from coal-burning power plants. Prior to her work at WVU, Dr. Babyak was an AmeriCorps member, and worked with coal mine drainage in southwestern Pennsylvania. Dr. Babyak received her Bachelor's degree from Saint Vincent College, in Latrobe, PA, where she was mentored by Dr. Caryle Fish. Dr. Babyak has been at Appalachian since August, 2004.

Research in Dr. Babyak's group centers around environmental analytical chemistry and environmental monitoring. Students in Dr. Babyak's group spend time both in the lab developing analytical methods and in the field collecting samples. Current projects include development of an analytical method to quantify environmental endocrine disruptors in water samples and investigation of the effects of the Tennessee Valley Authority (TVA) coal ash spill on water quality and aquatic life in the Emory River. Research ideas suggested by students are also welcomed and encouraged.

### **Dr. Nicole Bennett**

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Dr. Bennett teaches Organic Chemistry I and II and Fundamentals of Organic Chemistry. After receiving a B.S. in Chemistry at UNC-Chapel Hill, she earned a Ph.D. in Organic Chemistry from the University of Wisconsin- Madison in 1996 under the supervision of Edwin Vedejs. Dr. Bennett wrote her graduate thesis on *Probing the Origins of Stereoselectivity for the Wittig Reaction of Stabilized Ylides*. Following graduate school, Dr. Bennett taught Organic Chemistry at Hope College in Holland, MI for many years. She happily left the mid-west to become a

professor at Appalachian in the Fall of 2002. **Dr. Bennett is currently serving as a Program Director at NSF in Washington, DC.**

Dr. Bennett has three ongoing research projects that involve synthesis of small molecules that may have important pharmacological properties. They are as follows: 1) Total synthesis of taxane diterpenes using  $\pi$ -allyl palladium chemistry. 2) Microwave-induced preparation of substituted pyridines and 3) Formation of allylic ethers using the inverse electron-demand Diels-Alder Reaction.

**Dr. Claudia Cartaya-Marin**

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Dr. Claudia Cartaya-Marin is an organic synthetic chemist interested in developing synthetic methods and in the total synthesis of natural products that possess anti-cancer properties. She obtained her B.S. in Chemistry from Universidad Simon Bolivar in Caracas, Venezuela, and then came to the United States, where she got her Masters at Northeastern University, working on organo-metallic chemistry. She then joined the lab of Dr. Barry Snider at Brandeis University, in Waltham, MA, where, for her Ph.D. degree, she accomplished the total synthesis of (+)-nitramine, a proposed neurotoxin. She also studied Lewis acid-catalyzed reactions of aldehydes, and developed a novel cyclization reaction.

After completing her Ph.D., she accepted a post-doctoral position in the Chemistry Department at Cornell University, where she worked on the total synthesis of biosynthetic intermediates of the shikimic acid pathway. Since arriving at Appalachian State University in 1986, she has extended her research to include the one pot synthesis of 5,7-diphenyl-2,3-Dihydro-1 H-pyrrolizine; the study of the reactions of sodium hydrogen selenide with  $\alpha,\beta$ -unsaturated compounds and the synthesis of enaminones using Lewis acids as activators.

Currently, Dr. Cartaya-Marin is studying the nucleophilic aromatic substitution reaction of trihalogenated benzenes with cyclic amines, as well as the use of microwaves to enhance organic reactions. She is also collaborating with Dr. Ece Karatan from the Biology Department on a project that involves the synthesis of cyclic-diguanylic acid and using this acid to find the cyclic-diguanylic acid (c-di-GMP) regulated signal transduction pathways in the bacterium *Vibrio cholerae*.

Her teaching responsibilities have included Biochemistry, Advanced Organic Chemistry, Organic Synthesis, and Organic Chemistry I and II lectures and laboratories. She is currently teaching Fundamentals of Organic Chemistry.

Students in her lab obtain experience performing literature searches; learn proper research notebook keeping and the use of modern synthetic techniques. They use chromatographic techniques to separate and purify products and use NMR and IR spectroscopy and GC/MS to characterize the compounds that they synthesize.

**Dr. Brooke E. Christian**

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Dr. Christian graduated from Appalachian State University in 2005 and received her Ph.D. in Biological Chemistry in 2010 from the University of North Carolina at Chapel Hill. Her graduate work in the research group of Dr. Linda Spremulli focused on mechanisms of translation initiation in mammalian mitochondria. Brooke did her postdoctoral work at Yale University as an NIH postdoctoral fellow in the laboratory of Dr. Gerald Shadel where she studied the contribution of mitochondrial reactive oxygen species to the neurodegenerative disease Ataxia-Telangiectasia. Dr. Christian joined the department of chemistry at Appalachian State University in 2015 and teaches biochemistry and biochemistry lab.

Current research projects in the Christian lab are focused on mitochondrial reactive oxygen species and the roles they play in assembly of oxidative phosphorylation complexes and in adipocyte differentiation. Techniques used in the Christian lab include tissue culture, western blotting, qPCR, PAGE (denaturing/SDS and blue native), shRNA knockdown of genes of interest, immunofluorescence, and subcellular fractionation.

**Dr. Megen A. Culpepper**

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Dr. Culpepper received her Ph.D. in Analytical Chemistry in 2009 from the University of Kansas working in the research groups of Dr. Julian Limburg and Dr. Emily E. Scott. Her graduate work focused on determining the structure and function of a prolyl 4-hydroxylase-like protein involved in collagen production. After graduate school, Dr. Culpepper moved to Northwestern University to the laboratory of Dr. Amy C. Rosenzweig where she was awarded an NIH postdoctoral fellowship studying biological methane oxidation by the membrane protein particulate methane monooxygenase. Dr. Culpepper

joined the department of chemistry at Appalachian State University in 2014 and teaches classes in Analytical and Introductory Chemistry.

Current research projects in the Culpepper lab utilize interdisciplinary techniques encompassing biochemistry, molecular biology, and analytical chemistry. Research projects investigate the protein structure and biochemical function of enzymes involved in the global sulfur cycle. Namely, an enzyme responsible for the degradation of dimethyl sulfide (DMS), the major contributing volatile organic sulfur compound (VOSC) in our atmosphere implicated in climate regulation. Research students learn protein expression and purification as well as biochemical characterization using analytical instrumentation

**Dr. Michael Hambourger**

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Dr. Hambourger joined the faculty at Appalachian State University in 2009. He received his Ph.D. from Arizona State University, under the tutelage of Dr. Thomas A. Moore; followed by a one-year postdoctoral appointment in the same laboratory. Dr. Hambourger's graduate and post-doctoral work focused on photochemical charge-separation in organic/inorganic hybrid systems, proton-coupled electron transfers as related to photochemical reactions, and coupling biological catalysts with electrodes for technological applications.

Dr. Hambourger teaches introductory chemistry and is establishing a new research laboratory at Appalachian State University which is aimed at developing first-row transition metal catalysts suitable for water oxidation, hydrogen production, and/or carbon dioxide reduction. His laboratory is exploring low-cost materials and processing techniques for the electrodeposition of suitable catalysts, with the hope of identifying candidates for renewable energy storage at an appropriate scale. Further, Dr. Hambourger is exploring the interface between single electron photochemical events and multi-electron/multi-proton catalytic reactions, in hopes of better understanding (and mimicking) the process of natural photosynthesis.

Students in the research laboratory are exposed to the fundamentals of electrochemistry and photochemistry, as well as to several spectroscopic techniques used to characterize the materials produced. Students are encouraged to make significant contributions to laboratory research, while developing the skills, self-discipline, and confidence necessary for a successful scientific career.

**Dr. Jennifer Perry Cecile**

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Dr. Perry received a Ph.D. in Chemistry in 2003 from Duke University working in the research group of Dr. John Simon. Her graduate research used fluorescence spectroscopy to characterize photophysical properties of the fungal metabolite ochratoxin a and to examine the binding of various ligands to the blood protein human serum albumin. After graduate school, Dr. Perry completed postdoctoral research at the National Institute of Environmental Health Sciences in the Research Triangle Park, NC. During that time, she studied structure/function interactions of negatively charged xenobiotics and a family of proteins named the organic anion transporters (OATs). She also became interested in the effects of genetic variability and regulation on OAT protein expression and function.

Dr. Perry joined the chemistry department at Appalachian State University in 2007 teaching introductory and physical chemistry courses. Currently, her research involves techniques from biochemistry, biophysical chemistry and biology. Her research projects include implementing a nematode model system to study xenobiotic transport by OATs, building models of OAT structure to analyze amino acids that contribute to OAT function, and observing functional consequences of genetic splice variants and single nucleotide polymorphisms on OAT protein expression and regulation.

**Dr. Libby Puckett**

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Dr. Puckett has been teaching Introductory, Analytical, and Forensic Chemistry classes at Appalachian State University since the fall of 2004. She holds a Ph.D. in Bioanalytical Chemistry from the University of Kentucky under the guidance of Dr. Leonidas G. Bachas and Dr. Sylvia Daunert. Her research involved the development of sensing systems for clinical and pharmaceutical applications. Dr. Puckett received her Bachelor's degree from Eastern Kentucky University in Forensic Science in 1996.

Although she is a bioanalytical chemist by training, her research looks at problems from different perspectives. Her research crosses many disciplines, including forensic science, molecular biology, and electrical engineering, but ultimately utilizes analytical chemistry as the unifying science. The current research projects in her laboratory have two main concentrations – forensic analysis and biological applications. Currently, there are three different instruments being used to study forensic samples. The first project involves using capillary electrophoresis (CE) to separate compounds of forensic interest, including drugs, explosives, and inks/dyes. The second project entails the comparison of solid phase extraction techniques (activated charcoal strips (ACS), solid phase microextraction (SPME) “needles”, and the Gerstel Twister) for the analysis of arson accelerants. Comparisons will be performed on the gas chromatograph (GC). The final project utilizes the gas chromatograph-mass spectrometer (GC-MS) for the detection and quantification of cocaine on U.S. and foreign currency.

There are currently three projects for the analysis of biological entities. The first project involves using a custom-made capillary electrophoresis system in conjunction with chemiluminescence detection for the determination of enzyme kinetics using a technique called enzyme mediated microanalysis (EMMA). The second project is the creation of a homogeneous protein-based assay for the detection of organophosphates by utilizing a fusion protein between organophosphorus hydrolase (OPH) and enhanced green fluorescent protein (EGFP). This assay will allow us to monitor the hydrolysis of organophosphates found in pesticides and chemical warfare agents. The third project involves creating

a whole-cell sensor, containing a fusion protein between  $\beta$ -lactamase and EGFP, to monitor the rate at which  $\beta$ -lactam antibiotics (penicillins) cross cell membranes. This will aid in determining the bioavailability of possible new drug candidates or inhibitors of  $\beta$ -lactamase.

### **Dr. Michael Ramey**

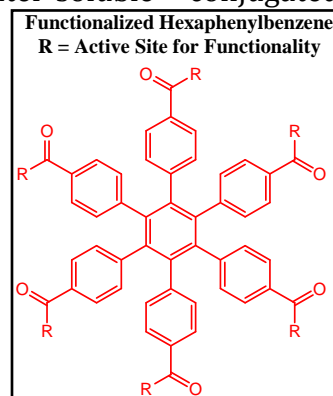
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Dr. Ramey teaches a variety of organic chemistry classes at Appalachian State University. He holds a Ph.D. in organic chemistry from the University of Florida under the guidance of Dr. John Reynolds. His research involved the synthesis and characterization of water-soluble conjugated polymers for light emission applications. Prior to his work at UF, Dr. Ramey attended Virginia Polytechnic and

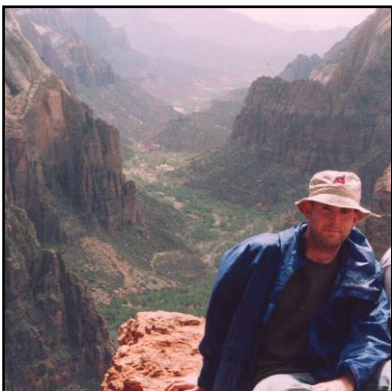
State University where he worked with Dr. Judy Riffle on high temperature polymers. Following graduate studies, he worked as a researcher for the Air Force Research Laboratories at Wright-Patterson AFB, Dayton, Ohio, until his appointment at Appalachian in August 2002.

Currently, Dr. Ramey's research centers on the use of organic synthetic techniques to construct molecules for the controlled release of fragrances and the assembly of charged species for ionic conduction. The materials under development have potential in fuel cell/battery membranes and stimuli activated scent release applications. Students are exposed to three principles of research: self-discipline, in-depth synthetic knowledge / planning, followed by experimental design and execution. Input and new ideas from students are always encouraged and expected.



**Dr. Al Schwab**

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Dr. Schwab received his Ph.D. in Polymer Science from The University of Akron and his B.S. in Materials Science and Engineering from the University of Illinois at Urbana-Champaign. His main research interests include the development of metallic nanoparticles as broadly applicable photocatalysts, computational studies of nanometer-scale self-assembly, and the development of novel rubber materials.

When illuminated with laser radiation, metallic nanoparticles have the ability to enhance light intensity at the surface of the particle. When these particles are dispersed in a system of photochemical reagents, the light intensity enhancement can lead to an overall increase in the reaction rate. Like conventional catalysts, the nanoparticles would not be consumed in the course of the resulting chemical reaction. Unlike conventional catalysts, the nanoparticles can catalyze any photochemical reaction rather than reactions involving specific reactants. A student project in this area involves the synthesis of metal nanoparticles, characterization of particles with electron microscopy, and quantification of photochemical rates upon laser exposure.

Self-assembly, a process wherein molecules assemble into larger-scale objects is an important component of biological structure formation as well as a vital tool in the burgeoning field of nanotechnology. In general, intermolecular attractive interactions drive molecular assembly and entropy counters assembly. One quickly realizes, however, that these thermodynamic counterparts are rather limited in their ability to control the overall size of any given assembly. To address these issues of assembly size control, computational studies will be implemented to determine the limits of thermodynamic size control and to devise assembly design strategies using computational evolution algorithms. A student project in this area will involve programming of Monte Carlo simulations and computer analyses of simulation results.

Rubber materials are typically composed of long chain molecules that are covalently cross-linked to one another. These covalent cross-links impart the material with the ability to reversibly stretch to great lengths, but also remove the material's ability to be recycled. By altering the chemical nature of the cross-links between the polymer chain molecules, these materials can be made recyclable. The unique cross-linking chemistry also offers several possibilities for developing rubber materials that act as sensors to various stimuli. A student project in this area will include the synthesis of new polymeric materials and their subsequent optical and mechanical characterization.



### **Dr. Nicholas Shaw**

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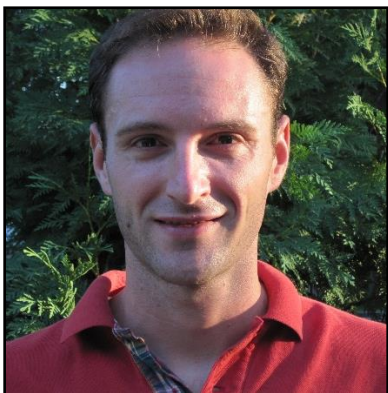
Dr. Shaw joined the faculty at Appalachian State in 2015. He received his B.A. in chemistry and mathematics from St. Olaf College in 2002. Upon completion of his undergraduate degrees, he attended graduate school at Clemson University, working in the laboratory of medicinal chemistry under the guidance of Dr. Dev P. Arya and received his Ph.D. 2010. His graduate work focused on the development and synthesis of new aminoglycoside therapeutic agents. Following his graduate work, Dr. Shaw accepted a position as visiting assistant professor at The College of Wooster. From

2011-2015, Dr. Shaw taught courses in introductory chemistry, organic chemistry and medicinal chemistry and mentored 17 undergraduate research assistants.

Currently, Dr. Shaw teaches courses in organic chemistry. The Shaw Research Group focuses on the development of new synthetic methodologies. Traditionally, synthetic organic reactions are dependent on the energy, orientation, and velocity of the reactants in solution. The difficulty associated with controlling these variables have historically resulted in increased reaction times, decreased reaction yield, and decreased purity. Students in the Shaw Research Group have recently developed new synthetic methodologies that circumvent traditional synthetic pitfalls and increase reaction yield and purity while decreasing reaction time.

### **Dr. Bob Swarthout**

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Dr. Swarthout is an analytical environmental chemist. His research applies the techniques of analytical chemistry to study environmental issues of local and global concern. He received a Ph.D. in Earth Systems Science from the University of New Hampshire where his doctoral research focused on the air quality impacts of hydraulic fracturing for natural gas. He also conducted postdoctoral research at Woods Hole Oceanographic Institution studying the environmental impacts of major oil spills including the Deepwater Horizon disaster. He currently teaches Introductory

and Capstone courses in Environmental Chemistry and Environmental Science. Dr. Swarthout's research focuses on the environmental impacts of naturally produced organic compounds and organic pollutants derived from fossil fuel production on air quality, water quality, and climate. One current research project involves measuring volatile organic compounds and other trace gases at the Appalachian Atmospheric Interdisciplinary Research (AppalAIR) atmospheric observatory in order to better understand the complex relationship between

emissions of volatile organic compounds (VOCs) from trees and shrubs and climate. The thousands of VOCs produced by plants can influence our climate because they can form aerosols which reflect incoming solar radiation and because they can compete for reaction with radical species that control the lifetime of greenhouse gases. Another project involves investigating the chemical weathering of oil spills. Oil is a complex mixture of thousands of organic compounds and the composition of spilled oil changes over time in the environment. The goal of this research is to understand how these changes affect the environmental fate and toxicity of these weathered oil residues.

Students working on these projects will gain hands-on experience working with the analytical instrumentation used in atmospheric and environmental chemistry. They will also develop skills in scientific communication through the presentation and publication of their findings. Most importantly they will work to provide much needed information about pressing environmental issues that will help shape ongoing policy debates.

**Dr. Brett Taubman**

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Dr. Brett Taubman teaches analytical and environmental chemistry as well as fermentation science and introductory chemistry courses. He received his Ph.D. in Chemistry from the University of Maryland in 2004 under his dissertation advisor Dr. Russell Dickerson. His graduate work focused on the meteorological and dynamical impacts on regional air quality, specifically with respect to aerosol optical properties, as measured from a light aircraft. Following his graduate studies, Dr. Taubman worked as a Research Associate in The Pennsylvania State University Department of Meteorology with his research advisor Dr. Anne Thompson. There he designed and operated a mobile atmospheric chemistry laboratory to investigate global air pollution transport and validate satellite retrievals of atmospheric pollutants.

As co-founder of the Appalachian Atmospheric Interdisciplinary Research (AppalAIR) facility and through on-going collaborations with NASA and NOAA, his current research interests are focused on the relationships between aerosol chemical and optical properties and their impacts on the regional climate. Additionally, as part of an interdisciplinary research team in fermentation sciences, he performs applied research in bio-processing of agricultural and industrial waste streams, water treatment, and environmental remediation as well as in designing innovative approaches for reducing resource utilization and improving operating efficiencies in the campus fermentation pilot plant.

**Dr. Dale Wheeler**

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Dr. Wheeler teaches introductory and inorganic chemistry classes at Appalachian State University. He holds a Ph.D. in inorganic chemistry from the University of Idaho under the guidance of Dr. Leszek Czuchajowski. His research involved the synthesis and characterization of organometallic salts as model systems for nonlinear optical materials. Prior to his work at UI, Dr. Wheeler attended Kansas State University where he worked with Dr. Eric Maatta on vanadium imido complexes. Following graduate studies, he completed a postdoctoral fellowship at

Berea College as a Henry and Camille Dreyfus Fellow and then was a faculty member at the University of Wisconsin – Parkside until his appointment at Appalachian in August 1998.

Currently, Dr. Wheeler's research centers around the use of organic and air-sensitive organometallic synthetic techniques to create molecules that are potential nonlinear optical materials. The noncentrosymmetric crystallization of these chromophores is an essential requirement for efficient second-order nonlinear optical properties. The research has applications for optical and electro-optical devices in the telecommunications and optical data-processing industries. Research students learn synthesis and purification techniques, characterization methods, and how to formulate experimental design.

**Dr. Steve Williams**

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Chemistry is controlled by the behavior of the electrons in materials. Since the early 1930's the equations that describe the motions of electrons have been known, and the solution of these equations should allow accurate prediction of almost every aspect of chemical behavior, including properties of individual molecules, thermochemistry ( $\Delta H$ ,  $\Delta S$ , and  $\Delta G$ ) and kinetics of chemical reactions, and even the behavior of solutions and other types of chemically interesting bulk matter. Unfortunately, while the equations are known, their exact solutions are not. This means that the prediction

of chemical behavior must be based on approximate solutions. The equations come from detailed treatments of atoms, molecules, and bulk matter using the methods of quantum mechanics. The approximate solutions come from numerical computations carried out on large computers with sophisticated computer programs.

In the recent past students who have worked on computational projects with Dr. Williams have studied such diverse subjects as boron and aluminum halides, aromatic nucleophilic substitution reactions, rhodium dimer homogeneous catalysts, relativistic effects in rhodium acetate, and Raman spectroscopy. These studies have resulted in publications and presentations at regional and national professional meetings.

The computational projects of most current interest are related to the chemistry of combustion, which is a very large and technologically important field. There is a quite peculiar bit of chemistry that occurs in the initial (low temperature) combustion of most fuels: "negative temperature coefficient." In the vast majority of chemical reactions, an increase in temperature causes an increase in reaction rates. However, in many combustion reactions the opposite occurs over a small temperature range. If the rate is plotted as a function of temperature the onset of the negative temperature coefficient (NTC) regime appears as a local maximum in the plot.