Reed College Chemistry Department Research Interests

Juliane Fry (Atmospheric Chemistry)

Research in my lab is focused on measuring the chemical composition of atmospheric particulate matter (aerosol) in the Portland area, correlating observed trends and patterns with other facets of the local chemistry (O3, NOx, black carbon) and meteorology, and analyzing air quality effects on atmospheric particle formation using chemical kinetics models and satellite datasets. The Columbia River Gorge will continue to be a focus of our measurements, as well as Portland's urban chemistry.

At a practical level, individual projects can focus on: (1) further development of aerosol collection and functional group analysis protocols, employing FTIR, NMR or GC-MS analytical techniques; (2) modeling regional atmospheric chemistry to determine interesting locations for future field measurements, either developing kinetics box models in Matlab or running a large-scale regional chemistry/meteorology model (WRF/Chem), run on the PNNL supercomputer; or (3) analyzing available aerosol and NOx global data spatial/temporal trends to seek correlations that elucidate the chemistry of aerosol formation. Finally, we have a laboratory environmental simulation chamber for the measurement of gas/aerosol reactions, so laboratory work on a "synthetic atmosphere" is also possible.

Dan Gerrity (Physical Chemistry)

My students and I apply new techniques in laser spectroscopy to the study of chemical reaction dynamics, molecular electronic structure, and analytical chemistry. Specific research topics include; resonance Raman studies of the electronic structure and bonding in Group 6 metal hexacarbonyl complexes, investigations of the multiphoton dissociation dynamics of gas phase chromium carbonyl complexes using atomic fluorescence spectroscopy, and building an LIBS (Laser-Induced Breakdown Spectroscopy) instrument at Reed.

Maggie Geselbracht (Inorganic Chemistry)

Research projects in my lab are related to new materials for energy production and storage. In one project, we are investigating the electrochemical properties of V2O5 gels for use as cathodes in lithium ion batteries. V2O5 gels are prepared by the hydrolysis and condensation reactions of vanadium alkoxides in the form of bulk monoliths and transparent films on conducting substrates. These transparent electrodes can be used to explore structure property relationships and the influence of defects on the lithium ion storage behavior. The second project involves highly collaborative work searching for new photocatalysts that will split water using solar energy and efficiently produce hydrogen from a renewable energy source. The ideal photocatalyst will likely be a mixed metal oxide combining a number of different metal cations to enhance various features of the catalyst. Initially, combinatorial libraries of metal oxide films of varying composition are screened for the best potential "hits," followed by more detailed analysis of the structure and composition of potentially active materials.

Arthur Glasfeld (Biochemistry)

My work is focused on understanding the structural basis for metal ion specificity in biochemistry. Transition metals, including manganese, iron, cobalt, copper nickel and zinc are trace nutrients found in virtually all cells. It is essential that each metal find its way to the correct cellular site in order to promote necessary functions. Projects in my lab are typically geared towards proteins involved in metal ion homeostasis in bacteria, including transcriptional regulators and transporters. Students are engaged in cloning genes for novel targets, purifying proteins and characterizing their structure and function through a variety of biophysical techniques, including fluorescence spectroscopy and x-ray crystallography.

Sarah Kliegman (Inorganic Chemistry)

Halocarbon polluted waters pose risks to both human health and the environment. The goals of the research in our group are to: identify and characterize model systems with which to study the mechanisms of attenuation of emerging target compounds; optimize conditions to achieve maximum degradation of target compounds; and determine mechanisms for reactions of metal-complex with target compounds. There are several types of experiments inherent to this research. A thesis project in my group will include several experiment types, including:

- Synthesis and characterization (^{1}H- and ^{13}C-NMR, UV-vis, electrochemistry, X-ray crystallography) of ligands and metal complexes.

- Reactivity assays and chemical analysis (HPLC, GC-MS, NMR) to assess scope of reactivity.
- Kinetic studies and optimization of reaction conditions.
- Mechanistic studies to identify reaction intermediates and elucidate interactions between the metal complex and the organic substrate.

Rebecca LaLonde (Organic Chemistry/Organometallic Chemistry)

Research in my group is aimed at developing new catalytic reactions that are not only highly selective but also have minimal environmental impact. While many modern catalysts are composed of rare, expensive and potentially toxic metals, our work is focused on developing new organometallic catalysts based on bismuth, a cheap, readily-available, recyclable and non-toxic element. Projects range from designing and synthesizing novel bismuth complexes, testing the catalytic activity of these complexes, to demonstrating the utility of bismuth in the synthesis of complex natural products.

Alan Shusterman (Computational Chemistry/Green Chemistry)

I am working on multiple projects involving different aspects of computational chemistry, particularly those that will bring useful modeling tools to a larger audience. Recent projects have included: · Collaboration with Wavefunction, Inc. (www.wavefun.com) on the development of new software products such as ***iSpartan*** (available for iPad and iPhone on the iTunes store)

- Development of new conceptual/theoretical models for use in research and education, e.g., qualitative and quantitative valence bond (VB) models (see "A Chemist's Guide to Valence Bond Theory" by S.S. Shaik & P.C. Hiberty)
- Structure determination by NMR spectroscopy using experimental and calculated spectra (see "Stereochemistry and Mechanism of the Ring-Opening Reaction of Cyclopropylenones with LiCu(Me)2" *Organometallics*, **2012**, *in press*, DOI:10.1021/om300520r)
- Molecular modeling of green oxidation catalysts such as Fe-TAML complexes (T. Collins, Carnegie Mellon University)