This summer the Carleton Chemistry Department will offer its continuing summer research program for Carleton students. We expect to offer research positions to between eight and twelve new students. For the most part, the new student researchers will come from the sophomore and junior classes. Professors Burand, Chihade, Gross, Hofmeister, Hollingsworth, and Kohen will offer projects that reflect their research interests. These projects are financially supported through external grant agencies and Carleton College. The research projects offered by each faculty member will be presented briefly at the Friday, January 11, Chemistry Department Seminar in Olin 04 at 3:30 p.m. and are described in the following document. We strongly encourage you to attend this seminar if you are at all interested in doing research in the department this summer.

**Dates of the Program:** Monday, June 16, through August 22, for a total of 10 weeks. Each student will arrange starting and ending dates and summer vacation with his or her professor; these dates are often flexible.

**Stipend:** $4,200 for 10 weeks.

**Expectations of Students by the Chemistry Department:**
A research position in our summer research program is a full-time position. You should not plan on taking a second job during the same period.

Each week you will be expected to attend a research conference with all of our summer researchers. Once or twice during the summer you will give an oral presentation on your project. If you would like, you may have the opportunity to give a presentation on your research at state or national research meetings in the future. Following the summer of research, you will prepare a comprehensive written report and give a poster on your research at the fall All Science/Math Student Poster Session at Carleton.

**Deadlines and How to Apply:** By Monday, January 28, submit a one-page description of your interests and background to the Chemistry Department’s Administrative Assistant, Wendy Zimmerman. List the three professors you would like to work with in order of preference. Also tell us how strong your preferences are and how flexible you are in accepting a position in all three groups. In addition to attending the January 11 seminar, you should talk to individual professors in order to explore your interest in their research project. Keep in mind that some professors will not invite a student to join their research group unless the student has taken the time to stop by, meet the professor, and discuss the research project.

On Monday, February 25, offers will go out to individual students in campus mail. We will ask for your decision on our offer by Monday, March 10 (the last day of classes).

**Reasons to Participate in the Summer Research Program:** Research is considered by many to be at the pinnacle of intellectual endeavors as it is the main vehicle by which new knowledge is created. Research requires a demanding combination of intellect, creativity, endurance, and curiosity. Many valuable skills are developed in the research laboratory. Some examples
include the ability to work as a member of a team, to operate sophisticated instrumentation, and to use available resources to become a life-long learner. Research is also excellent preparation for graduate school, a career in the medical sciences, or a career in other scientific or quantitative fields.

Choosing to do research at Carleton offers a number of advantages. First of all, you will have the chance to get to know your professors much better. In addition, you can start preparing for your summer research experience during spring term. This additional preparation will improve the quality of the research you can perform during the short ten-week summer. Furthermore, if you wish, your research project can be continued as an independent study during the following academic year. Some students at Carleton who have had the most positive research experiences have worked on their research projects over the course of two years. Unlike the experience at a larger institution, colleges like Carleton offer research opportunities exclusively for undergraduate students. At a larger institution, you would probably work most directly with a graduate student or postdoc, which is a good, yet different kind of experience. At Carleton you are guaranteed to work closely with a professor and to have your peers as research colleagues.

Life at Carleton and in Northfield is much different during the summer than during the academic year. You will be surprised by the pace, and you will be pleased to know that you will not need your down jacket and face mask (you may want to buy a fan). Many of the facilities (such as the gym, pools, weekly movies, etc.) at Carleton are open for summer programs. We will have at least two expeditions; canoe trips, baseball games, Valley Fair, and tubing have been popular choices in the past.
The area of organic electronics has expanded tremendously in the past few years. My recent graduate and post-doctoral research has focused on the design of organic materials for use in thin-film transistors. Traditionally, semiconductors are fabricated from inorganic materials such as silicon; however, many different organic compounds have been found to exhibit semiconducting behavior. One of my goals is to synthesize new compounds in this field, with emphasis on the characterization of these compounds. Characterization will include studies with NMR, UV-vis, cyclic voltammetry, and mass spectrometry. Additionally, X-ray crystallography and device testing will be conducted in collaboration with the University of Minnesota.

I would like to recruit one or two students to do research this summer. The research will involve synthesis of new molecules, as well as characterization of these molecules with the techniques listed above. It is important to note that this is a five-week research program. Students who are interested should contact me to set up a meeting to discuss the details.
Professor Joe Chihade
Aminoacyl-tRNA synthetases (aaRSs) play a central role in the translation of genetic information. These enzymes, which are essential in all living organisms, catalyze the formation of an ester linkage between amino acids and the specific transfer RNAs (tRNAs) that bear the corresponding anticodons. The specific matching of particular amino acids with particular tRNAs is the basis of the genetic code. As molecular matchmakers, aaRSs must discriminate between very similar tRNA molecules, using a set of unambiguous intermolecular interactions to choose only their cognate substrate. Although all organisms may have an aaRS for a particular amino acid-tRNA pair, the specific enzyme-tRNA interactions can vary from organism to organism. For example, the mitochondria of animals contain tRNAs that are described as “bizarre”. These tRNAs differ both in shape and in sequence from those found in all other forms of life. Understanding how aaRSs interact with and recognize these aberrant tRNAs is the main focus of my research.

The particular enzyme we study is human mitochondrial alanyl-tRNA synthetase (Hs mt AlaRS), the enzyme responsible for linking alanine to tRNA

Ala. We have two complementary aims: (1) Find out what part or parts of human mitochondrial tRNA

Ala are recognized by the enzyme, and (2) find out what part of parts of human mitochondrial AlaRS interact with the tRNA specifically. Our major approach to Aim #1 is to test various tRNAs that differ from human mitochondrial tRNA

Ala in significant ways to find out what differences block alanylation. By comparing the tRNAs that work with those that don’t, we’ll be able to identify the pieces of tRNA that are most important for the interaction. Our approach to Aim #2 is to produce truncation mutants, in which we delete portions of the AlaRS protein sequence. These enzyme fragments will then be tested for their ability to alanylate or bind tRNA

Ala. If an enzyme fragment doesn’t function, we’ve removed something important. Much progress has been made on both of these goals, so we can now draw a schematic description of the interaction, as shown in the figure at right, but work remains to be done to add detail to this picture.

Techniques used in my lab include protein purification, in vitro transcription of mutant and wildtype tRNAs, creation of new RNA and protein mutants using site-directed mutagenesis, enzymatic assays to measure charging ability, and probing of tRNA structures to determine regions of protein-RNA interactions. I plan to take 1-3 new students in my lab this summer.
Professor Deborah Gross

“So Many Particles, So Little Time!”

The air around us is full of aerosol particles (small droplets or chunks of solids), which impact our lives in many ways. These particles come from natural as well as anthropogenic (human) sources. They nucleate cloud droplets, they decrease visibility by scattering sunlight, and they impact our health when we inhale them. Our research group works with an Aerosol Time-of-Flight Mass Spectrometer (ATOFMS), code-named “Gromit,” to obtain size and chemical composition of the aerosol population in real time. With this data, we hope to try to increase our understanding of some of the complex issues in the atmosphere. The types of issues we are interested in include:

- Mechanisms for formation of secondary organic aerosol (SOA) in the atmosphere.
- Emissions from combustion of biofuels.
- Analysis of complex aerosol datasets using new data analysis strategies.

I hope to recruit two to three new students this summer to work at Carleton. Students working in my lab will get an opportunity to work on analysis of ATOFMS data sets obtained in collaboration with groups at the University of Minnesota, University of Wisconsin, and the Paul Scherrer Institute in Switzerland. We have long-standing collaborations with these groups, and have a number of complex data sets to work with. Our analysis is done using software under development by Dave Musicant’s group in the CS Department at Carleton. Our work in Summer 2008 will involve analysis of data from a variety of studies. In addition to working with existing data sets, we will obtain data here at Carleton to search for and improve our understanding of macromolecules in the ambient air.

**IF YOU ARE INTERESTED IN JOINING THESE PROJECTS, YOU SHOULD DO ALL OF THE FOLLOWING THINGS:**

- Come talk to me as soon as possible, to discuss the details of the research and to see the ATOFMS instrument. I won’t accept anyone into the group unless we’ve talked about your interests, the projects, etc.
- Be prepared to for the possibility of spending part of the summer away from Carleton. While we are not sure yet of our specific plans, fieldwork might well be part of them! Your expenses for fieldwork would be paid.
- Plan to enroll in independent studies (Chem 394) in Spring, 2008 as well as throughout the 2008-2009 academic year (except terms when you might be off campus) to work on this project.
**Professor Gretchen Hofmeister**

**Background**

Controlling the outcome of a particular transformation in a manner that produces a single product is of fundamental importance in organic synthesis. Synthetic targets, such as pharmaceutical agents, natural products and their derivatives, and polymers, are increasingly more complex, requiring that the methods used to accomplish specific transformations be more selective. One approach for controlling reactivity is to employ metal-ligand complexes as mediators or catalysts for organic transformations. Metal ligand complexes are useful because the metal can activate a substrate by coordination (thereby speeding up a desired reaction in comparison to undesired reactions), and the organic ligand can control the orientation of the substrate as it approaches the metal (thereby controlling the three-dimensional structure of the product).

My group has been investigating the coordination of trisphenols (Fig. 1A) to metals such as titanium(IV) and aluminum(III), in order to produce new chiral complexes that will stereoselectively promote carbonyl addition reactions and polymerization reactions. We envisioned that trisphenols 1a,b would be useful ligands for these metals because the sterically encumbered ligand would prevent dimerization of the metal complexes, resulting in more reactive catalysts. We expected that the ligand would adopt an asymmetric (S-shaped) conformation because a steric interaction between the terminal ortho substituents would prevent the ligand from adopting a symmetric (U-shaped) conformation (Fig. 1B). This asymmetry could then be useful for catalyzing stereoselective organic transformations. Finally, the trisphenol structure lends itself to preparation in chiral form, by the introduction of a methyl substituent at one ortho methylene carbon (1b, Fig. 1A). This methyl group should control the chirality of the ligand conformation, by avoiding the sterically congested metal center. When resolved into enantiomerically pure form, the ligand could be used to prepare enantioselective metal catalysts.

**Research Projects**

I plan to have one to two students in my group during the summer of 2008. I am planning to use the summer to finish up work that my group has been doing to understand the mechanism by which titanium trisphenolates initiate the polymerization of lactide to produce poly(lactic acid) (PLA), a biodegradable polymer. This summer’s work should enable us to complete a manuscript for publication in this area.

We have prepared and characterized titanium and aluminum complexes of chiral and achiral trisphenol (eqs 1, 2). We also learned that the titanium complexes we have prepared (3a, eq 1) promote the stereoselective ring opening polymerization (ROP) of lactide to produce a
biodegradable polymer, poly(lactic acid) (eq 3). The goal for this summer is to more completely characterize the structure of the active polymerization catalyst in solution. This will require careful kinetics studies that will be performed in NMR tubes at 80 °C with the rigorous exclusion of air and water. Additionally, we will collaborate with Andy Mobley, an NMR expert at Grinnell College, to do diffusion NMR experiments that will help us determine the molecular weights of the active polymerization catalyst.

This work involves air-sensitive synthesis using glove box and Schlenk line techniques, multinuclear and two-dimensional NMR spectroscopy, and polymer synthesis and analysis. Students who love to do synthesis and who are highly motivated to do rigorously careful laboratory work are a good fit for research in my group. Given the nature of this work, there is a strong possibility that evenings and weekends will be spent using long blocks of “NMR time.” Additionally, the collaboration with Andy may involve periodic travel to Grinnell College.

Overview of Basic Experiment

Photons from the laser are used to excite gas-phase organometallic compounds within chamber.

The timing of data collection is set by the time a detector reports that the laser beam has made it through the chamber.

Signal from the TOFMS is sent to the oscilloscope for collection.

My research program employs a powerful pulsed laser which can deliver different wavelengths in the visible and near ultraviolet through several wavelength-conversion techniques. The nanosecond laser pulse is focused down into the middle of a vacuum chamber and the incredible amounts of energy over such a short time accomplish the break-up of target gas molecules within the chamber. Ions that are formed when electrons are removed from the fragments are detected in a time-of-flight mass spectrometer (TOFMS). In one laser shot, the different fragments are identified by the time it takes for them to travel to the detector.

The way that energy is absorbed is different from anything you have so far encountered—a series of multiphoton process occurs where two or three photons (instead of the usual one) are absorbed at once to cause absorption between states. This multiphoton strategy allows us to study molecules with many chemical bonds due to the absorption of so much energy from the laser beam. Having tuneable visible and near-ultraviolet light is important since these colors correlate in energy with specific excited states that control different aspects of chemical reactivity.

The dissociative pathway taken is controlled by the nature of electronic excited states encountered along the way. This is the direct application in our work—namely, the study of how metal-metal bonds compete with metal-ligand bonds in the breakup. Detailed spectroscopic and electronic-energy knowledge for metal-containing molecules is lacking and even many basic questions have not yet been answered. Take for example manganese decacarbonyl, Mn$_2$(CO)$_{10}$, which is formally described through molecular orbital theory as having a Mn-Mn single bond. Photochemical experiments in the near-ultraviolet conducted in the gas phase and solution often disagree as to what the initial photofragments even are! Solution studies can be clouded by complex solvent interactions that take place after the photon has broken a bond yet it is in solution that the unique properties of these metal carbonyls will be put to use in accomplishing unique reaction chemistry. Gas phase data such as ours will help decipher the initial events to clarify the pathways.
Agreement is nonetheless converging on Mn$_2$(CO)$_9$ and Mn(CO)$_5$ as the primary fragments in the near-UV photolysis of Mn$_2$(CO)$_{10}$ although details of their relative importance at different wavelengths are still unclear. A paper by Ferraudi$^1$ reporting results in solution tried to correlate these fragments with the nature of the excited states but the correlation was not great. This research question is good for our group to take on since the relative simplicity of the gas phase data coupled with our additional wavelength tuneability should help pin down the correlations to specific excited states and will provide the primary focus for the summer.

There is no way to get a full sense of the types of experiments you would do by reading this introduction or listening to a short overview talk. For starters, the pictures above show you a few key components. The best way is to come and see the laboratory for yourself and see if this type of research could be right for you. In addition to the laser, vacuum, and mass-spectrometric techniques mentioned above, other skills that you would naturally acquire in performing this type of research include controlling equipment by computers using LabView software, understanding how to use oscilloscopes and photodetectors, thinking a lot about molecular orbitals, and working with a wide range of tools to accomplish these tasks. I will be taking probably one but at most two students into the group this summer.

Two views of Mn$_2$(CO)$_{10}$:

**Professor Dani Kohen**

I am a theoretical and computational physical chemist. I am interested in the general area of dynamics in condensed phase (how atoms and molecules move and interact when they're not by themselves). Currently, I am using atomistic simulations to understand and characterize at the molecular level how small gas molecules interact with pure CO₂ on molecular sieve's pores, and how this interaction changes in the presence of other gases that are present in our atmosphere. The goal of these studies is to provide a basic understanding of the use of molecular sieves as filters to remove CO₂ from the atmosphere. In recent years the power of computational research has been shown to provide scientific insight that might not result from experimental research alone.

This research will introduce students to the study of chemistry through the lens of molecular simulations, which provide a powerful tool in giving new meaning to familiar concepts. It will also serve as a reference point to understand not only the computational chemistry literature but also why the importance of this field as a tool for studying many problems keeps growing.

The way my research group works is that I mostly write the programs (software), my student collaborators use and modify these to investigate chemical systems; and then, together, we use the results to learn about the chemical processes that occur in the systems we study. This is exactly what my group, David Selassie ('09) and Felix Amankona-Diawuo ('08) have been doing for a year and a half now. In doing this kind of research the learning curve is steep, but the results are very satisfying and my student collaborators made significant progress in their own projects while enjoying doing research. I anticipate that I will be able to invite two or three students to join my group. If you are interested in joining us, please stop by to talk to me and even better, ask a member of my group about their experience as their thoughts will be the best introduction to our work.