BOSTON COLLEGE

GRADUATE SCHOOL OF ARTS AND SCIENCES

CHEMISTRY

A MESSAGE FROM THE CHEMISTRY FACULTY AT BOSTON COLLEGE

Welcome to the Chemistry Department at Boston College. We hope that you will take this opportunity to learn more about our dynamic research community. Our department is made up of nearly 200 scientists studying all phases of contemporary chemical science, including many interdisciplinary areas interfacing with the fields of biology, medicine, physics, and materials science. Over 120 graduate students, 40 undergraduate majors and 25 postdoctoral fellows work hand in hand with approximately 20 internationally recognized and acclaimed faculty members advancing the frontiers of chemistry. In addition, we host a diverse seminar series that brings outstanding visiting scientists from around the world to the department annually for formal and informal interactions with all members of the department.

Recent achievements of the scientists in the Chemistry Department reflect the exciting research culture we enjoy. In the last year, over 100 research papers were published by BC chemists in internationally recognized journals, and the overwhelming majority of these papers were co-authored by our graduate students. Boston College is especially proud to be ranked among the top 10 university chemistry departments worldwide with respect to the impact that the scientific publications of its faculty and students have on the frontiers of research, as measured by the number of citations per paper over the period 1995-2006. Each year, we celebrate the accomplishments of our students with our Graduate Student Research Symposium, a daylong event featuring seminars and poster presentations by our graduate student colleagues.

Many of our graduate students have obtained prestigious fellowships, including those sponsored by the American Chemical Society, the Department of Education, the National Institutes of Health, the National Science Foundation, the Department of Energy, NASA and the pharmaceutical industry. In addition, graduates of the department have gone on to assume positions of scientific leadership in private industry as well as in some of the finest academic institutions in the world.

For a genuine appreciation of the exciting atmosphere of the department and the outstanding facilities that provide the setting for our research, we strongly encourage you to visit us both through our website and its links, and in person. We would be happy to arrange individual meetings with faculty and students so that you can get a firsthand sense of the vibrant scientific environment of our department. For more information please e-mail us at chemadmissions@bc.edu.

GRADUATE STUDIES

COURSEWORK

First-year course requirements provide the student with a breadth of knowledge in the traditional fields: organic, chemical biology, physical chemistry and inorganic chemistry. While a specific number of credits is not required for the Ph.D. degree, each student is encouraged to pursue a program of studies, with the approval of his/her advisor consistent with his/her individual educational goals.

SELECTION OF A RESEARCH ADVISOR AND AN ORIGINAL RESEARCH PROJECT

During the first semester of graduate studies, students meet with faculty members and advanced graduate students to explore the dissertation project opportunities available in different research groups. The Graduate Student Research Symposium, typically held in October, showcases the research of our graduate students in a day-long event that consists of oral and poster presentations. The symposium is an excellent opportunity for new graduate students to learn more about research activities in the department. By the end of the first semester, most students have selected a research advisor and identified a potential dissertation project that they will begin investigating in the second semester.

TEACHING REQUIREMENTS

Some teaching or equivalent educational experience is required. This requirement may be satisfied by at least one year of service as a teaching assistant or by suitable teaching duties. Arrangements are made with each student for a teaching program best suited to his/her overall program of studies. Waivers of teaching requirements may be granted under special circumstances with the approval of the Chemistry Department.

PH.D. CANDIDACY AND COMPREHENSIVE EXAMINATIONS

At the end of the second year, Ph.D. students must pass an oral candidacy exam that stresses material from their own research specialty and other related areas. Members of the student's dissertation committee (usually selected at the beginning of the second year) comprise the exam committee. Ph.D. students must pass 8 cumulative examinations that test the student's critical awareness and understanding of the current literature.

PH.D. DISSERTATION AND DEFENSE

The Ph.D. degree requires a dissertation based upon original research, either experimental or theoretical. For the Ph.D. candidate, a research project requiring three to four years of sustained effort will begin usually after the first year of study. An oral defense of the dissertation before a faculty committee completes the degree.

FINANCIAL ASSISTANCE

First-year graduate students typically receive financial support as teaching assistants during the academic year. Teaching assistants serve as instructors in undergraduate laboratories or act as leaders of discussion sections in the classroom. For lab TAs, teaching responsibilities include six to eight hours of contact time with the students per week as well as grading lab reports. Discussion TAs attend class lectures, oversee four one-hour discussion periods per week and assist in grading quizzes and exams. Teaching assistantships carry a ten-month stipend.

Tuition remission scholarships (non-taxable) are also awarded to graduate students to cover the complete cost of tuition for the program requirements.

Financial support, during the summer of the first year and continuing throughout the period of graduate study, is available to students in the form of either research or teaching assistantships. Research assistantships are provided by individual professors from existing research grants, while teaching assistants are supported from departmental funds. Summer RA stipends cover two months salary. The average yearly stipend for 2009 - 2010 is $24,500.

STUDENT PROFILES

Our graduate students come from across the United States and the globe. The demographics of our graduate program varies, but currently it is 55% male, 45% female, and includes 45% international students. While some students enroll in the Boston College Chemistry Ph.D. program immediately following their undergraduate studies, others begin their Ph.D. studies after working in a chemistry-related industry.

GRADUATE RESEARCH SYMPOSIUM

Every October, the research activities of the BC Chemistry Department are showcased during the Graduate Research Symposium. This event features seminar and poster presentations made by our graduate students. The Graduate Research Symposium is a highlight of the academic year, as it includes reports of the most exciting advances made in BC Chemistry research groups during the preceding year.

FREE FOOD FRIDAY

Several times a year, the department faculty and graduate students gather for a relaxing meal or other organized events. For example, frequently we enjoy food catered by a local restaurant and the company of colleagues. This event is a great opportunity to catch up with members of other laboratories and to meet newcomers to the department.

Admissions

ADMISSION REQUIREMENTS

The deadline for the receipt of applications for fall admission is January 2. Applicants apply through he Graduate School of Arts and Sciences. Please visit www.bc.edu/gsas for information on how to apply and links to the application form.

The following documents are required as part of the application packet:

- Statement of Purpose: include area(s) of research interest (organic, bioorganic, chemical biology, inorganic, theoretical, computational, physical, and biophysical). Additionally, include specific research faculty with whom you might be interested in as a future advisor.

- Graduate Record Examination (GRE) send official scores with your application materials. The institution number is 3083.

- GRE Subject Test in Chemistry: required for graduates of foreign universities and highly recommended for all.

- Three letters of recommendation from professors or supervisors. It is highly recommended that at least one letter be from an academic source.

- Transcripts showing required courses: those normally required for a BS degree in chemistry, biochemistry, or chemical biology.

- TOEFL Report: Students who speak a native language other than English must provide evidence of English proficiency. A score of 550 on the paper-based test, 213 on the CBT test (computer-based test), or 79 on the new iBT test (internet-based test) or higher on the Test of English as a Foreign Language (TOEFL) is required. Remember to enter the Boston College School Code 3083 to ensure that the score report is sent to us, student copies or photocopies of TOEFL scores are not accepted.

DEPARTMENT OPEN HOUSE

The department invites students accepted to the Chemistry Ph.D. program to visit the department to talk with faculty and students. While on campus, students will have the opportunity to learn about the cutting-edge research being conducted in the department and other aspects of the curriculum. We also offer tours of the facilities and the Boston College campus.

Research Instrumentation and Facilities

The Chemistry Department is housed in the 109,000 square-foot Eugene F. Merkert Chemistry Center, with modern classrooms, research laboratories, computation, instrumentation, and facilities all in a single building. Ongoing renovations and upgrades ensure that our resources are kept up-to-date. The Merkert Center's sophisticated research facilities include: a Mass Spectrometry facility with electrospray and MALDI-TOF mass spectrometers; a high-field Nuclear Magnetic Resonance (NMR) facility, featuring 300 MHz, 400 MHz, and 500 MHz NMR spectrometers; and an X-ray crystallography facility. Our facilities are run by full-time professional scientific staff.

Each faculty member has participated in the design of his or her laboratory, built to accommodate state-of-the-art instrumentation and to provide flexibility for changing research needs. For example, an X-ray crystallography laboratory is fully equipped with a diffractometer and area detector, constant temperature rooms for crystal growth, and several VAX and silicon graphics computers for investigation of protein and small molecule structures. ESR spectroscopy, stopped-flow kinetics equipment, preparative centrifuges, scintillation counters, a DNA synthesizer, lasers, and ultra-high vacuum apparati are also available for use by individual research groups.

Other departmental instrumentation includes ReactIR, UV-Vis, atomic absorption, circular dichroism, GC-mass spectroscopy, gas and high performance liquid chromatography, magnetic susceptibility, electrochemistry, fermentation, and DNA-and protein-sequencing equipment. Faculty research collaborations with several area institutions afford our graduate students and postdoctoral staff easy access to additional state-of-the-art instrumentation.

Boston College is deeply committed to advancing research instrumentation and facilities in accordance with its strategic plan for strengthening the physical and life sciences. For example, a state-of-the-art clean room has recently become available. Significant new research instrumentation is planned for the Chemistry Department in the areas of chemical biology, X-ray, and advanced laser spectroscopy.

Seminar Series

We host a diverse seminar series that brings outstanding visiting scientists from around the world to the department annually for formal and informal interactions with all of the members of the department. Weekly seminars highlight nationally recognized speakers in organic, inorganic, physical and biological chemistry. In addition, the seminar series is highlighted by our annual University Lectureship, which invites acclaimed scientists to the department for a three-day visit highlighted by stimulating, daily seminars. Our recent University Lecturers include:

2008-2009	Jay D. Keasling, University of California at Berkeley
2007-2008	Peter G. Wolynes, University of California at San Diego
2006-2007	Richard R. Schrock, Nobel Laureate, MIT
2005-2006	Paul A. Wender, Stanford University
2004-2005	James Wells, President and CEO, Sunesis Pharmaceuticals
2003-2004	Stephen R. Leone, University of California, Berkeley
2002-2003	Robert H. Grubbs, California Institute of Technology
2001-2002	E. J. Corey, Nobel Laureate, Harvard University
2000-2001	Christopher Walsh, Harvard Medical School

Industrial Recruiting Program

Every year the department manages an Industrial Recruiting program that brings companies to the Merkert Chemistry Center to interview eligible students for post-degree job opportunities. This program is available to all undergraduate and graduate students in the chemistry and biochemistry majors at Boston College. Graduate students who are in their final year of study may participate during their search for permanent positions as well as undergraduates who are seeking summer internships or research associate positions. When industrial laboratories visit the Chemistry Department, their recruiter/scientist typically gives a presentation, conducts individual interviews with students, and meets/lunches with faculty. The recruiting schedule runs from September through December for Ph.D. candidates and January through March for BS candidates.

A few of the corporate partners who recruit at BC include, but are not limited to, Schering-Plough, Amgen, Merck, Novartis, Abbott Labs, AstraZeneca Sepracor, Roche, Millennium and Pfizer. For more information regarding this program, please contact the Graduate Program Administrator at 617-552-1735.

THE FACULTY

WILLIAM H. ARMSTRONG, ASSOCIATE PROFESSOR

Ph.D. Stanford University, 1983
NIH Postdoctoral Fellow, Massachusetts Institute of Technology, 1983-1985

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Alfred P. Sloan Foundation Fellowship 1990; Presidential Young Investigator, NSF, 1988; Searle Scholar 1986

RESEARCH INTERESTS

Transition metal complexes function as homogeneous catalysts in a wide variety of systems of biological and industrial importance. Professor Armstrong is involved in the development of catalytically-active species placing emphasis on those that operate at the oxidizing and reducing extremes of the redox scale. He is particularly interested in multi-electron transformations. An example of a process under investigation that requires a highly oxidizing species is the conversion of water to dioxygen, as carried out in photosynthetic organisms at a center which contains a cluster of four manganese atoms as well as one calcium atom. At the other extreme of the redox scale, Professor Armstrong seeks highly reducing species capable of fixation of small molecules such as N_2, H_2, CO, and CO_2. Nitrogenase is an enzyme that employs a $MoFe_7$ metal cluster to catalyze the conversion of dinitrogen to ammonia. His approach to elucidation of the enzyme active site structures involves synthesis of novel transition metal clusters whose properties may be compared to those of the native system. An ideal biomimetic complex will not only reproduce the structural and spectroscopic properties of the enzyme but will also be able to function as the enzyme does. After more is understood about the enzyme active site structure and function via the biomimetic approach, Professor Armstrong hopes to optimize the performance of artificial catalysts and to extend, or in some cases restrict, their substrate specificities.

SELECTED PUBLICATIONS

- "Transition Metal Cluster Complexes for Dinitrogen Reduction" Armstrong, W. H.; Abu-Sbeih, K. (The Trustees of Boston College, USA). PCT Int. Appl., 2006, 30 pp.
- "Tuning Tetranuclear Manganese-Oxo Core Electronic Properties: Adamantane-Shaped Complexes Synthesized by Ligand Exchange" Christopher E.Dubé, Sumitra Mukhopadhyay, Peter J. Bonitatebus, Jr., Richard J. Staples, William H. Armstrong, *Inorganic Chemistry* 2005, 44, 5161-5175.
- "Manganese Clusters with Relevance to Photosystem II" Mukhopadhyay, S.; Mandal, S. K.; Bhaduri, S.; Armstrong, W. H. *Chem. Rev.* 2004, 104, 3981.
- "Shape-Shifting Tetranuclear Oxo-Bridged Manganese Cluster: Relevance to Photosystem II Water Oxidase Active Site" Mukhopadhyay, S.; Mok, H. J.; Staples, R. J.; Armstrong, W. H. *J. Am. Chem. Soc.* 2004, 126, 9202.
- "Illumination with Ultraviolet or Visible Light Induces Chemical Changes in the Water-soluble Manganese Complex, $[Mn_4O_6(bpea)_4]Br_4$" Antal. T. K., Lo, W., Armstrong, W. H., Tyystjärvi. E., *Photochemistry and Photobiology* 2009, published on-line, DOI: 10.1111/j.1751-1097.2008.00502.x.

STEVEN D. BRUNER, ASSOCIATE PROFESSOR

Ph.D., Harvard University, 2000
Postdoctoral Fellow, Harvard Medical School, 2000-2003

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Camille and Henry Dreyfus New Faculty Award, 2003; Damon Runyon Scholar Award, 2004-2006; NSF CAREER Award, 2007.

RESEARCH INTERESTS

Structurally complex natural products, such as the medicinally relevant antibiotics vancomycin and erythromycin, are biosynthesized by large, macromolecular enzyme assemblies. These assemblies frequently orchestrate difficult and interesting chemical transformations to construct diverse molecular scaffolds. Our research group will use the tools of synthetic organic chemistry, enzymology and structural biology to dissect the mechanism of these systems. A detailed understanding of the biosynthesis of natural products will be extended to the development of new synthetic methodology and to the engineering of biological systems to produce novel molecules with desired properties.

SELECTED PUBLICATIONS

- Widboom, P. F., Fielding, E. N., Liu , Y., Bruner, S. D. "Structural basis for cofactor-independent dioxygenation in vancomycin biosynthesis" *Nature*, 2007, 447, p. 342-345.
- Christianson, C. V., Montavon, T. J., Festin, G.M., Cooke, H. A., Shen, B., Bruner, S. D. "The mechanism of MIO-based aminomutases in beta-amino acid biosynthesis. " *J. Am. Chem. Soc.*, 2007, 129, p.15744-15745.
- Christianson, C. V., Montavon, T. J., Van Lanen, S. G., Shen, B., Bruner, S. D."The structure of L-tyrosine 2,3-aminomutase from the C-1027 enediyne antitumor antibiotic biosynthetic pathway" *Biochemistry*, 2007, 46, p. 7205-7214.

MICHAEL J. CLARKE, PROFESSOR

Ph.D., Stanford University, 1974

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NIH Young Investigator Award 1977-1980; NSF Program Director for Inorganic, Bioinorganic and Organometallic Chemistry, 2001-2004 and 2005-2008; Editor, Topics in Bioinorganic Chemistry, 1999-present; Editor, Structure and Bonding, 1984-1999; Co-Organizer of the first Metals in Medicine Gordon Conference, 2001. NIH Biometallic Study Section Member 1992-1997.

RESEARCH INTERESTS

The interactions of transition metal ions with biological molecules is important for understanding metalion function in the body and metaliophranc. The new knowledge learned is applied to the development of metallopharmaceuticals. For example, glutathione, which occurs in millimolar concentrations in cells, can either facilitate or hinder DNA binding by transition metal anticancer agents. Transferrin, which transports Fe^{3+} in the blood, also serves as a Trojan horse to provide some metal ions, such as Ru^{3+}, preferential entry into tumor cells. Some ruthenium complexes appear to be selectively toxic to tumors by being activated by reduction by the tumor itself to bind to nucleic acids. Ruthenium complexes

induce new modes of hydrolysis and oxidation, which may cut or otherwise damage DNA. The paramagnetism of Ru(III) also affects the NMR resonances of coordinated nucleotides so as to probe molecular orbital interactions. Applying sensitive electrochemical techniques to Ru-DNA adducts reveals that this metal can migrate within the DNA as a function of its oxidation state. Such interactions point toward the development of new transition metal agents bound to transferrin and then activated by the tumor to interfere with its DNA metabolism and possibly induce cell death by apoptosis.

Metallonitrosyls can be used as prodrugs for the in vivo release of nitric oxide, which exhibits many functions in the body including those as: a neurotransmitter, an enzyme activant, and a cytotoxic agent. My laboratory has been engaged in the synthesis of new complexes that should release NO in vivo and so possibly affect the biological activities mediated by this molecule, particularly those involving short term memory in the hippocampal section of the brain.

SELECTED PUBLICATIONS

- Krogh-Jespersen, K.; Stibrany, R. T.; John, E.; Westbrook, J. D.; Emge, T. J.; Clarke, M. J.; Potenza, J. A.; Schugar, H. J., Solid-State Changes in Ligand-to-Metal Charge-Transfer Spectra of (NH3)5RuIII(2,4-dihydroxybenzoate) and (NH3)5RuIII(xanthine) Chromophores. *Inorg. Chem.* 2008, 47, (21), 9813-9827.
- Holanda, A. K. M.; da Silva, F. O. N.; Sousa, J. R.; Diogenes, I. C. N.; Carvalho, I. M. M.; Moreira, I. S.; Clarke, M. J.; Lopes, L. G. F., Photochemical NO release from nitrosyl RuII complexes with C-bound imidazoles. *Inorg. Chem.* Acta 2008, 361, (9-10), 2929-2933.
- Haney, W.; Clarke, M.J., "Cheating on Tests: Prevalence, Detection, and Implications for Online Testing", book chapter in *Psychological Perspectives on Academic Cheating*, Anderman, E.A. and Murdock, T., eds, 2007, Elsevier, San Diego.
- Lopes, L. G. F., Castellano, E. E., Ferreira, A. G., Davanzo, C. U., Clarke, M. J., & Franco, D. W., "Reactivity of trans-[Ru(NH3)4P(OEt)3NO]X3 (X = PF6-, CF3COO-): modulation of the release of NO by the trans-effect", 2005, *Inorganica Chimica Acta*, 358(10), 2883-2890.
- Clarke, M. J., "Ruthenium Metallopharmaceuticals", Coord. *Chem. Rev.*, 2003, 236, 207-231.

PAUL DAVIDOVITS, PROFESSOR

Ph.D., Columbia University, 1964

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Fellow of the American Physical Society; R.W. Wood Prize, 2000; Boston College Distinguished Senior Research Award, 2001; Alpha Sigma Nu Book Award, 2003; AAAS Fellow.

RESEARCH INTERESTS

Interactions of gas molecules with liquid droplets in clouds and fogs play a fundamental role in many atmospheric processes such as acid rain formation, ozone depletion, and the formation of cloud condensation nuclei. Until recently experimental techniques or the study of interactions of gases with liquids were not available. Over the past several years in a joint program with Aerodyne Research Inc., we have developed accurate experimental techniques that make it possible to study various aspects of such interactions. The basic approach in all our studies is to bring gas molecules in contact with a liquid surface and then to examine how the gas enters the liquid, how it leaves it, and what chemical reactions occur at the gas-liquid interface. Results of our studies have been used to model atmospheric processes. However, gas-liquid interactions are of interest in other areas as well, notably in biochemical systems in which one finds gases interacting with liquids at cell boundaries.

For another related set of studies we have developed techniques for sampling and analyzing aerosols found in the atmosphere. Such aerosols have been shown to have important effects on climate and present serious health hazards. Their control is of important international concern. In a recent field study a researcher from the Boston College group and our Aerodyne research partners conducted a field studies in New York and Mexico City measuring pollutant emissions. The data from this study will play a role in formulating pollution control measures.

SELECTED PUBLICATIONS

- "CCN Activation Experiments with Adipic Acid: Effects of Particle Phase and Coatings on Soluble and Insoluble Particles. Silke S. Hings, William C. Wrobel, Eben S. Cross, Douglas R. Worsnop, Paul Davidovits, and Timothy B. Onasch. *Atmos. Chem. Phys.* 8 3735-3748, 2008.
- "Morphology Based Particle Segregation by Electrostatic Charge" Rajan K. Chakrabarty, Hans Moosmüller, W. Patrick Arnott, Mark A. Garro, Jay G. Slowik, Eben S. Cross, Jeong-Ho Han, Paul Davidovits, Timothy B. Onasch, and Douglas R. Worsnop", *J. Aerosol Science*, 39, 785-792, doi:10.1016/j.jaerosci.2008.04.008, 2008.
- "Chemical and Microphysical Characterization of Ambient Aerosols with the Aerodyne Aerosol Mass Spectrometer" Canagaratna, M. R., Jayne, J. T., Jimenez, J. L., Alfarra, M. R., Allan, J.D., Zhang, Q., Onasch, T. B., Drewnick, F., Coe, H., Middlebrook, A., Delia, A., Williams, L. R., Trimborn, A. M., Northway, M. J., DeCarlo, P.F., Kolb, C. E., Davidovits, P., Worsnop, D. R. *Mass Spectrometry Reviews*, 26, 185-222, (2007)
- "A novel method for estimating light-scattering property of soot aerosols using a modified single-particle soot photometer." R. S. Gao, J. P. Schwarz, K. K. Kelly, D. W. Fahey, L. A. Watts, T. L. Thompson, J. G. Slowik, P. Davidovits, and D. R. Worsnop. *Aerosol Science & Technology* 41, 125-135, 2007.
- ""Inter-Comparison of Instruments Measuring Black Carbon Content and Optical Properties of Soot Particles" Slowik, Jay G., Cross, Eben S., Han, Jeong-Ho, Davidovits, Paul, Onasch, Timothy B., Jayne, John T., Williams, Leah R., Canagaratna, Manjula R., Worsnop, Douglas R. Chakrabarty, Rajan. K., Arnott, William P. Schwarz, Joshua. P., Gao, Ru-Shan, Fahey, David W. Kok, Gregory. L. Baumgardner, Darrel G. *Aerosol Science & Technology*, 41, 295-314, 2007.
- "The Spectroscopy and Dynamics of Microparticles, Concluding Remarks," Paul Davidovits, Faraday Discuss., *DOI*: 10.1039/b711018a, 2007.

TORSTEN FIEBIG, ASSISTANT PROFESSOR

Ph.D., University of Gottingen, 1996
Postdoctoral Fellow, California Institute of Technology, 1997-1999

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Otto-Hahn Medal (Max-Planck Society), 1997; Dieter-Rampacher Award, (Max-Planck Society), 1997; DFG Postdoctoral Fellowship, 1997; Emmy-Noether Fellowship, 2000.

RESEARCH INTERESTS

At the present time my research group is interested in a fundamental understanding of molecular interactions and ultrafast processes (e.g. energy, electron and proton transfer) in complex molecular architectures.

Our primary focus is to develop and apply new spectroscopic methodologies for probing real-time structural changes in biological systems. The underlying goal is to understand molecular function by probing structure and dynamics simultaneously.

Currently, my group investigates the interaction of UV-radiation with DNA on the ultrafast time scale addressing the question of how electronic excess energy delocalizes and dissipates in p-stacked nucleic acids.

SELECTED PUBLICATIONS

- "Crossover from Superexchange and Hopping Mechanisms for Photoinduced Charge Transfer in DNA Conjugates", Lewis, F. D.; Zhu, H.; Fiebig, T.; Raytchev, M.; Wang, Q.; Shafirovich, V. *J. Am. Chem. Soc.* 2006, 128, 791-800.
- "Ultrafast Energy Transfer and Structural Dynamics in DNA", Trifonov, A.; Raytchev, M.; Buchvarov, I.; Rist, M.; Barbaric, J.; Wagenknecht, H. A.; Fiebig, T. *J. Phys. Chem.* B 2005, 109, 19490-19495.
- "Real-Time Spectroscopic and Chemical Probing of Reductive Electron Transfer in DNA", Kaden, P.; Mayer-Enthart, E.; Trifonov, A.; Fiebig, T.; Wagenknecht, H.-A. Angew. *Chem. Int. Ed.* 2005, 44, 1636-1639.
- "Femtosecond probing of the excited state absorption and structural relaxation in biphenyl derivatives", Mank, D.; Raytchev, M.; Amthor, S.; Lambert, C.; Fiebig, T. *Chem. Phys. Lett.* 2003, 376, 201-206.

JIANMIN GAO, ASSISTANT PROFESSOR

Ph.D., Stanford University, 2004; Postdoctoral Fellow, The Scripps Research Institute, 2004-2007.

Stanford Graduate Fellowship, 2001-2004; Smith Family Young Investigator Award, 2007-2009.

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RESEARCH INTERESTS

Proper folding of proteins is essential for their biological functions. In contrast, misfolding and aggregation of proteins have been implicated in a wide array of diseases, such as Alzheimer's disease and Prion Diseases. The primary research endeavor of our group is directed to understand the underlying mechanisms of protein folding and misfolding. A multidisciplinary approach, integrating organic chemistry, protein engineering and biophysics, will be employed to probe the physio-chemical basis of protein folding/misfolding processes. Detailed understanding of protein folding mechanisms will provide guidelines for protein structure prediction and design of unnatural functional polymers. Knowledge on protein misfolding will enable us to understand the pathologies of protein misfolding diseases and foster novel therapeutic strategies for disease treatment.

SELECTED PUBLICATIONS

- Hong Zheng, Kristofer Comeforo and Jianmin Gao, "Expanding the Fluorous Arsenal: Tetrafluorinated Phenylalanines for Protein Design", *J. Am. Chem. Soc.* 2009, 131, 18-19.
- Jianmin Gao, Daryl A. Bosco, Evan T. Powers, and Jeffery W. Kelly, "Localized Thermodynamic Coupling between Hydrogen Bonding and Microenvironment Polarity Significantly Stabilizes Proteins", *Nat. Struct. Mol. Biol.*, 2009, 16, in press.
- Jianmin Gao and Jeffrey W. Kelly, "Towards Quantification of Protein Backbone-Backbone Hydrogen Bonding Energies: An Energetic Analysis of an Amide-to-Ester Mutation in an α-Helix within a Protein," *Protein Science*, 2008, 1096-1101.

AMIR H. HOVEYDA, JOSEPH T. AND PATRICIA VANDERSLICE MILLENNIUM PROFESSOR AND CHAIR OF THE DEPARTMENT

Ph.D., Yale University, 1986; American Cancer Society Postdoctoral Fellow, Harvard University, 1987-1990

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NSF Young Investigator Award, 1992; Pfizer Award in Synthetic Organic Chemistry, 1993; Alfred P. Sloan Research Fellowship, 1994; Camille Dreyfus Teacher-Scholar Award, 1994; Novartis Lectureship Award, 1997; American Chemical Society Cope Scholar Award, 1998; Boston College Distinguished Senior Faculty Research Award, 2000; ExxonMobil Excellence in Catalyis Award, 2002; NIH MERIT Award, 2005.

RESEARCH INTERESTS

Our research group is primarily concerned with the design and development of new selective transformations and their application to total synthesis of complex molecules of biological significance. We are keen on the discovery of reactions that are enantioselective, which require inexpensive and non-toxic starting materials and which are catalytic. We are particularly interested in developing processes that do not have precedence in classical organic chemistry. The addition of Grignard reagents to unactivated alkenes, catalytic enantioselective olefin metathesis, catalytic asymmetric Strecker amino acid synthesis, and Cu-catalyzed conjugate additions are representative of some of the new and unique transformations that have recently been developed in our group.

Our interest in new reaction development is accompanied by a strong commitment to an understanding of related mechanistic principles. It is through our knowledge of reaction mechanisms that we hope to introduce new reagents and unusual modes of reactivity. However, we are aware that combinatorial chemistry and high-throughput screening is an exciting way to discover new catalytic processes. In fact, our group was one of the first to utilize such principles in developing efficient asymmetric

reaction (Ti-catalyzed addition of TMSCN to epoxides). These exciting new strategies are routinely utilized in our research.

We appreciate that the true test of the utility of a new synthesis method is its usefulness in a total synthesis setting. Synthesis of complex natural products such as fluvirucin B and chloropeptin 1 that are of biological significance is therefore a critical part of our research activities. Our synthesis schemes are strongly dependent on the success of methods and pathways that have been designed and developed in our own laboratories.

SELECTED PUBLICATIONS

- "A New Class of Chiral Catalysts for Enantioselective Olefin Metathesis," S. J. Malcolmson, S. J. Meek, E. S. Sattely, R. R. Schrock, A. H. Hoveyda, *Nature* 2008, 456, 933.
- "Enantioselective Total Synthesis of Clavirolide C. Applications of Cu-Catalyzed Asymmetric Conjugate Additions and Ru-Catalyzed Olefin Metathesis," M. K. Brown, A. H. Hoveyda, *J. Am. Chem. Soc.* 2008, 130, 12904.
- "Lewis Base Activation of Grignard Reagents with *N*-Heterocyclic Carbenes. Cu-Free Catalytic Enantioselective Additions to *γ*-Chloro-*α,β*-Unsaturated Esters," Y. Lee, A. H. Hoveyda, *J. Am. Chem. Soc.* 2006, 128, 15604

EVAN R. KANTROWITZ, PROFESSOR

Ph.D., Harvard University, 1976; Postdoctoral Fellow, Harvard University, 1977

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Camille Dreyfus Teacher-Scholar Award, 1982; Alfred P. Sloan Research Fellowship, 1983; NIH Career Development Award, 1985.

RESEARCH INTERESTS

Work in my laboratory is centered around an understanding of the relationship between protein structure and function and in particular, how the protein structure relates to catalysis, metal binding and cooperativity in enzyme systems. Systems that are under investigation currently include aspartate transcarbamylase and dihydroorotase in pyrmidine nucleotide biosynthesis, and fructose 1,6- biophosphatase in the gluconeogenesis pathway. Aspartate transcarbamylase and fructose 1,6-bisphosphatase are control enzymes that are involved in the regulation of their respective metabolic pathways.

One of the most important questions in biochemistry today concerns how the cell's enzymatic reactions are coordinated and regulated on the molecular level. Since a number of diseases result when metabolic controls break down, a detailed knowledge cellular regulation is vital. In particular, our research is concentrating on the molecular details of how the actual protein molecules involved in the regulatory process function.

Inhibition of these regulatory molecules has the potential to be therapeutic drugs for a variety of diseases. For example, inhibitors that target aspartate transcarbamoylase and dihydroorotase of the malaria parasite have the potential to be new anti-malarial agents. While inhibitors of fructose 1,6-bisphosphatase have the potential to be anti-diabetic agents. In order to design new classes of inhibitors for these and other enzymes, we have developed a virtual high-throughput screening system. The system uses a cluster of computers to dock the structures of all commercially available compounds to the target receptor site, in order to identify potential inhibitors of the target enzyme.

In order to acquire a molecular-level understanding of the catalytic and regulatory functions of these enzymes, as well as how the inhibitors identified interact with the enzymes, we are involved in determining their three-dimensional structures by X-ray crystallography. These structures not only allow us to help understanding the catalytic and regulatory properties of these enzymes, but also to help in the design of second generation, even more potent inhibitors.

SELECTED PUBLICATIONS

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- "Trapping the Tetrahedral Intermediate in the Alkaline Phosphatase Reaction by Substitution of the Active Site Serine with Threonine," Wang, J., Kantrowitz, E. R., (2006) *Protein Sci.* 15, 2395-2401.
- "Direct Observation in Solution of Pre-existing Structure Equilibrium for a Mutant of Allosteric Aspartate Transcarbamoylase," Fetler, L., Kantrowitz, E. R., Vachette, P. (2007) *Proc. Natl. Acad. Sci. U. S. A.* 104, 495-500.
- "Structural Model of the R state of Escherichia coli aspartate transcarbamoylase with substrates bound." Wang, J., Eldo, J., and Kantrowitz, E.R. (2007) *J. Mol. Biol.* 371, 1261-1273.

T. ROSS KELLY, THOMAS A. AND MARGARET A. VANDERSLICE PROFESSOR

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National Institutes of Health Career Development Award, 1975; American Chemical Society Cope Scholar Award, 1996; Teacher of the Year Award Phi Beta Kappa (Boston College chapter) 2004; Fellow of the American Association for the Advancement of Science, 2007.

RESEARCH INTERESTS

Over the years, this research group has accomplished the total synthesis of approximately three dozen natural products. Individual natural products that we choose as targets range from structurally simple to complex. They are selected as objectives because their architectures are novel and have not been synthesized previously. Many also have important biological activities. Lactonamycin serves as a case in point, because it not only possesses an unprecedented structure but also because it has outstanding antibiotic activity against bacteria that are resistant to current antibiotics. Natural products whose synthesis we have completed of late include nigellicine, HKI 0231 and the antibiotics nostocine A and pseudoiodinine.

A second main area of research is the design and synthesis of what might be called molecular devices. The initial example was the first molecular brake. More recently, we reported the results of our studies on molecular "ratchets." We have now also devised a related system that achieves unidirectional

rotation. To wit, we have accomplished a prototype of a molecular motor by using the energy-rich chemical phosgene to power clockwise-only rotation in this molecule. Work is currently underway to optimize the system so that it rotates continuously and rivals the speed of its biological and mechanical counterparts.

Further areas of interest are molecular recognition and the process of self-assembly. Following the lead of biological systems that assemble spontaneously from their molecular components, we are seeking to develop sophisticated chemical systems that self-assemble from simpler pieces. Organic zeolites and other new materials are among the goals, with metal coordination and hydrogen bonding being the primary organizing forces we hope to harness.

SELECTED PUBLICATIONS

- T. R. Kelly (Editor) "Molecular Machines", Topics in Current Chemistry, Springer Verlag, *Heidelberg*, 2005, Vol. 262.
- T. R. Kelly, E. L. Elliott, R. Lebedev and J. Pagalday, "Synthesis of the Pyrazolo[4,3-e][1,2,4]triazine Family of Natural Products: Nostocine A, Fluviol A, and Pseudoiodinine." *J. Am. Chem. Soc.*, 128, 5646-5647 (2006).
- T. R. Kelly, X. Cai, F. Damkaci, S. B. Panicker, B. Tu, S. M. Bushell, I. Cornella, M. J. Piggott, R. Salives, M. Cavero, Y. Zhao, and S. Jasmin, "Progress toward a Rationally Designed, Chemically Powered Rotary Molecular Motor." *J. Am. Chem. Soc.*, 129, 376-386 (2007).
- M. D. Markey, Y. Fu, and T. R. Kelly, "Synthesis of Santiagonamine." *Org. Lett.*, 9, 3255-3257 (2007).

JASON S. KINGSBURY, ASSISTANT PROFESSOR

Ph.D., Boston College, 2002; NSF Predoctoral Fellow, Boston College, 1998-2001; NIH Postdoctoral Fellow, Harvard University, 2003-2006

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National Science Foundation Predoctoral Fellowship, 1998; Boston College Outstanding Graduate Student Award, 2002; NIH Postdoctoral Fellowship, 2003.

RESEARCH INTERESTS

Our goal is to apply the principles of transition metal catalysis to the asymmetric synthesis of highly functionalized, strained small molecules. Representative targets include substituted aziridines, cyclopropanones, cyclobutanones and cyclopropane amino acids. Such building blocks are ideal precursors for enantioselective total syntheses of new natural products.

The methods and reaction sequences we will develop are the result of careful retrosynthetic planning for selected complex molecules. In essence, we seek to merge a more classic (target-inspired) approach to organic synthesis with a keen awareness of the contemporary issues of practicality, efficiency, and selectivity.

Advances in this area will have meaningful downstream effects on society, including cheaper medicines and materials as well as decreased pollution and resource expenditure. From an educational standpoint, these projects in multi-step synthesis are a wonderful means for connecting students to the importance of chemistry in the world around them, while simultaneously refining characteristics such as dedication, perseverance, and creativity.

SELECTED PUBLICATIONS

- "Catalytic Homologation of Cycloalkanones with Substituted Diazomethanes. Mild and Efficient Single-Step Access to α-Tertiary and α-Quaternary Carbonyl Compounds," Moebius, D. C.; Kingsbury, J. S. *J. Am. Chem. Soc.* 2009, 131, 878-879.
- "Enantioselective Total Synthesis of Isoedunol and b-Araneosene Featuring Unconventional Strategy and Methodology," Kingsbury, J. S.; Corey, E. J. *J. Am. Chem. Soc.* 2005, 127, 13813-13815.
- "Regarding the Mechanism of Olefin Metathesis with Sol-Gel–Supported Ru-Based Complexes Bearing a Bidentate Carbene Ligand. Spectroscopic Evidence for Return of the Propagating Ru Carbene," Kingsbury, J. S.; Hoveyda, A. H. *J. Am. Chem. Soc.* 2005, 127, 4510-4517.
- "A Recyclable Ru-Based Metathesis Catalyst," Kingsbury, J.S.; Harrity, J.P.A.; Bonitatebus, P.J., Jr.; Hoveyda, A. H. *J. Am. Chem. Soc.* 1999, 121, 791-799.

DAVID L. MCFADDEN, PROFESSOR

Ph.D., Massachusetts Institute of Technology, 1972; Postdoctoral Fellow, Harvard University, 1972-1973; Alfred P. Sloan Research Fellowship, 1977.

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RESEARCH INTERESTS

My research involved kinetics and dynamics of free radical and electron attachment reactions in the gas phase. Currently I play an active role in the development of undergraduate curricular and research opportunity programs.

SELECTED PUBLICATIONS

- "Gas-Phase Atom-Radical Kinetics of Atomic Hydrogen, Nitrogen, and Oxygen Reactions with Fluoromethylene Radicals," Tsai; C. P.; McFadden, D. L. *J. Phys. Chem.* 1990, 94, 3298.
- "Electron Attachment Reactions of Perfluoroalkyl Transition Metal Carbonyls: Rate Constants and Product Analysis", Marotta, C. J.; Tsai, C. P.; McFadden, D. L. *J. Phys. Chem.* 1989, 91, 2194.
- "Kinetic Study of Electronically Metastable Nitrogen Atoms, N(2DJ), by Electron Spin Resonance Absorption", Fell, B.; Rivas, I.V.; McFadden, D. L. *J. Phys. Chem.* 1981, 85, 224.
- "Kinetics of the O + F2 reaction: a case of low reactivity of elemental fluorine", Krech, R. H.; Diebold, G. J.; McFadden, D. L. *J. Am. Chem.* Soc. 1977, 99, 4605.

LARRY W. MCLAUGHLIN, PROFESSOR

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American Cancer Society Faculty Research Award, 1991.

RESEARCH INTERESTS

Our primary research interests involve the understanding of the role(s) of weak interactions (ionic, hydrogen bonding and hydrophobic) in macromolecular complexes, primarily involving nucleic acids. These weak interactions often define three-dimensional structures that result in critical recognition events or in catalytic activity. To probe these interactions we employ organic chemistry to prepare analogue nucleosides or other non-nucleoside entities that are incorporated into DNA/

RNA sequences. If the presence of the analogue interferes (or enhances) a critical interaction, then a corresponding effect is observed in assays of binding efficiency or catalytic effectiveness. By understanding these interactions in greater detail, our ability to then selectively interfere with the macromolecular processes of DNA replication, transcription or translational provides an important opportunity for targeting viral infection and cancerous growth. Using this approach we are studying DNA-protein and DNA-ligand interactions, the recognition of triphosphates by polymerases, the ability to target DNA duplexes (or single stranded sequences) using a third strand to form triplexes, and more recently the construction of nanoscale structures based on DNA "arms" and "junctions" formed from metal-ligand complexes. Our long-term goals are to better understand macromolecular interactions and to use that knowledge to develop new types of pharmaceuticals, particularly antivirals.

SELECTED PUBLICATIONS

- D. Chen, Meena, S.K. Sharma and L.W. McLaughlin (2004) "Formation and Stability of a Janus-Wedge Type of DNA Triplex," *J. Am. Chem.* Soc. 126, 70-71.
- K.M. Stewart, J. Rojo and L.W. McLaughlin (2004) "Ru(II) Tris(bipyridyl) Complexes with Six Oligonucleotide Arms as Precursors for the Generation of Supramolecular Assemblies," Angew. *Chem. Int. Ed.* 43, 5808-5811.
- K. Zou, A. Horhota, B. Yu, J. Chaput, J.W. Szostak and L.W. McLaughlin (2005) "Synthesis of p-L-Threofuranosyl Nucleoside Triphosphates (tNTPs)" *Org. Lett.* 7, 1485-1487.

UDAYAN MOHANTY, PROFESSOR

Ph.D., Brown University, 1981; Postdoctoral Fellow, University of California at San Diego, 1981-1983; Postdoctoral Fellow, The University of Chicago, 1983 - 1985

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Westinghouse Science Talent Search Semi-Finalist; Max Planck Fellow; Japan Society of Promotion of Science Fellow; Research Corporation Award, Sigma Xi; IUPAC Award; Visiting Scientist, Dept. of Chemistry, MIT; Visiting Scholar, Lyman Laboratory of Physics, Harvard University; Visiting Scientist, Noyes Laboratory of Chemical Physics, California Institute of Technology; Visiting Professor, Okayama University; Visiting Professor, Dept. of Physics, University de Roma; Visiting Scholar, Dept. of Biochemistry and Molecular Biophysics, Columbia University; Visiting Scholar, Sloan Laboratory of Chemistry, Yale University; Davidson Institute Fellow Laureate Mentor Award; Siemens Westinghouse Foundation Outstanding Mentor Award; Visiting Scientist, Dept. of Physics and Applied Physics, Stanford University; Fellow, American Physical Society; Fellow, American Association for the Advancement of Science; Fellow, John Simon Guggenheim Memorial Foundation.

RESEARCH INTERESTS

My field of research is in theoretical and computational biophysics and chemical biology, and physical chemistry. Our interdisciplinary research program utilizes and develops a range of novel and powerful techniques that spans fields from modern physical chemistry, biophysics, biophysical chemistry and soft condensed matter physics. The driving force in the advances of our research program is due to our close collaboration with various experiment groups that enable us to test predictive nature of our models. A number of areas of current interest to us include (i) single molecule studies on the ribosome; ; nature of interaction of magnesium with the ribosome; (ii) chemical biology of DNA flexibility in vivo; (iii) dynamics of nucleic acid in gels; (iv) conformation order of random oligomeric RNA sequences; (v) equilibrium and dynamical properties of deeply supercooled liquids; (vi) development of stochastic process and field theoretical techniques to describe rare events.

SELECTED PUBLICATIONS

- Spasic, A.; Sitha, S.; Korchak, M.; Chu, S.; Mohanty, U. "Polyelectrolyte Behavior and Kinetics of Aminoacyl-tRNA on the Ribosome." *J. Phys. Chem.* B; 112, 4161 (2008).
- Casalini, R.; Mohanty, U.; Ronald, M. "A Thermodynamic Interpretation of the Scaling Dynamics in Supercooled Liquids." *J. Chem. Phys.* 125, 014505 (2006).
- Schultes, E.; Spasic, A.; Mohanty, U.; Bartel, D. "Structure Without Evolution: Acquisition of Compact Folds By RNA with Randomly Generated Sequences." *Nature and Structural Biology,* 12, 1130-1136 (2005).
- Taubes, C. H.; Mohanty, U.; Chu, S. "Ion Atmosphere Around Nucleic Acid." *J. Phys. Chem.* B 109, 21267-21272 (2005).

JAMES P. MORKEN, PROFESSOR

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Glaxo Smith Kline Scholars Award, 2001-2002; Astra-Zeneca Excellence in Chemistry Award, 2002; Bristol-Myers Squibb Award in Synthetic Organic Chemistry, 2002; David and Lucile Packard Foundation Fellow in Science and Engineering, 1998-2003; Alfred P. Sloan Research Foundation Fellowship, 2002-2004.

RESEARCH INTERESTS

Synthetic organic chemistry has undergone a paradigm shift over the past fifteen years with new metal-catalyzed transformations enabling bond formation in ways that chemists previously only dreamed about. Realizing the impact that new catalytic asymmetric reactions will have on the continued evolution of organic synthesis, we have focused our research on the development of new processes and on studying their utility in complex molecule synthesis. Our progress towards these goals depends upon expertise in many areas of chemistry including organometallic chemistry, physical organic chemistry, and synthetic organic chemistry.

Reactions of particular interest to our group are those that involve stereoselective transformations of simple unsaturated organic substrates. Along these lines, our group has recently developed the Rh-catalyzed enantioselective reductive aldol reaction and the Rh and Pd-catalyzed alkene diboration reactions. These processes enable the simple, selective and efficient construction of versatile chiral reaction products. To evaluate the utility of these processes we have engaged in the total synthesis of borrelidin, dihydroxanthatin, fraxinelone, subglutinol, and sclerophytin. These stereochemically and functionally complex structures provide a challenging proving ground for new methods and have also inspired new directions in the development of catalytic transformations.

SELECTED PUBLICATIONS

- "Pd-Catalyzed Tandem Asymmetric Allene Diboration/a-Aminoallylation." J. D.
- Sieber and James P. Morken. *J. Am. Chem. Soc.* 2006, 128, 74.
- "Palladium-Catalyzed Enantioselective Diboration of Prochiral Allenes." N. F. Pelz, A. R. Woodward, H. E. Burks, J. D. Sieber and J. P. Morken. *J. Am. Chem. Soc.* 2004, 126, 16328.
- "Enantioselective Total Synthesis of Borrelidin." M. O. Duffey, A. LeTiran and J. P. Morken, *J. Am. Chem. Soc.* 2003, 125, 1458.

MARY F. ROBERTS, PROFESSOR

Ph.D., Stanford University, 1974; Postdoctoral Fellow, University of Illinois, 1974-1975; NIH Postdoctoral Fellow, University of California at San Diego, 1975-1978

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Camille Dreyfus Teacher-Scholar Award, 1980; Alfred P. Sloan Research Fellowship, 1982; National Science Foundation Faculty Award for Women, 1992.

RESEARCH INTERESTS

Research in my laboratory centers on using a variety of physical techniques to define on a molecular level (i) how phospholipase and lipid phosphatase enzymes interact with interfaces, and (ii) the series of events triggered in cells by environmental stress, most notably salt and heat stress. For the first of these we are also developing a novel NMR technique ('high resolution ^{31}P NMR field cycling') to monitor dynamics of the phosphodiester region of the phospholipid and to identify types and time-scales of motion in vesicles and then to assess how protein interactions alter these parameters. The second research area has a metabolomics bias as well as a reliance on multidimensional experiments after introducing an NMR-active isotope into cells as a way of focusing on metabolite synthesis and turnover.

Phospholipases and lipid phosphatases are water-soluble enzymes that catalyze the hydrolysis of specific ester bonds in phospholipids. The products generated by these phospholipid lipases are often second messenger molecules that are components of cell signaling pathways. This implies tight control of these enzyme activities. Their phospholipid substrates are not monomeric but form a two-dimensional interface with components that can often regulate the enzyme by interacting at a site distinct from the active site. Our work is to define on a molecular level the complex interfacial behavior of two classes of phospholipid lipases: phosphatidylinositol-specific phospholipase C and PTEN, a tumor suppressor that specifically hydrolyzes phosphate esters at the C3 position of the inositol ring of phosphoinositides. NMR, fluorescence (including fluorescence correlation spectroscopy), and circular dichroism techniques are currently used in conjunction with mutagenesis and kinetic analyses to investigate how phospholipid substrates, interfacial activators, and inhibitors modulate the structure of each enzyme and how non-active site binding interactions are communicated to the catalytic site. Nearly all organisms respond to changes in external osmotic pressure (e.g., increased NaCl) by accumulating small molecular weight solutes, or osmolytes. Halotolerant archaea, models for life on early Mars or for life that might exist today in sub-glacial oceans of the Jovian moon Europa, possess unique osmolytes and moderately small genomes (many of which have been sequenced). We use in vivo and in vitro NMR techniques to identify and quantify these osmolytes in archaea, to deduce biosynthetic pathways for unusual solutes (e.g., ß-glutamate or di-myo-inositol-1,1'-phosphate), and to monitor molecular turnover under different conditions. This information allows us to identify and characterize key biosynthetic enzymes that can then be overexpressed in E. coli, and eventually should allow us to reconstruct the novel osmolyte pathways in that microorganism.

SELECTED PUBLICATIONS

- Sivanandam, V.N.; Cai, J.; Redfield, A.G.; Roberts, M.F. (2009) Phosphatidylcholine "wobble" in vesicles assessed by high-resolution ^{13}C field cycling NMR spectroscopy. *J. Am. Chem. Soc.* 131, 3420-3421.
- Wang, Y.K.; Chen, W.; Blair, D.; Pu, M.; Xu, Y.; Miller, S.J.; Redfield, A.G.; Chiles, T.C.; Roberts, M.F. (2008) Insights into the structural specificity of the cytotoxicity of 3-deoxy-phosphatidylinositols. *J. Am. Chem. Soc.* 130, 7746-7755.
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- Klauda, J.B.; Roberts, M.F.; Redfield, A.G.; Brooks, B.R.; Pastor, R.W. (2008) Rotation of lipids in membranes: MD simulation, 31P spin-lattice relaxation, and rigid-body dynamics. *Biophys. J.* 94, 3074-3083.
- Rodionov, D.A.; Kurnasov, O.V.; Stec, B.; Yan, W.; Roberts, M.F.; Osterman, A.L. (2007) Genomic identification and in vitro reconstitution of a complete biosynthetic pathway for the osmolyte di-myo-inositol-phosphate. *Proc. Natl. Acad. Sci. U.S.A.* 104, 4279-4284.

LAWRENCE T. SCOTT, LOUISE AND JIM VANDERSLICE AND FAMILY PROFESSOR

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NATO Senior Scientist Fellowship, 1981; Japan Society for the Promotion of Science Senior Scientist Fellowships, 1985 and 2003; Alexander von Humboldt Foundation Senior Scientist Award, 1999; Boston College Distinguished Senior Faculty Research Award, 2003; Elected Fellow, American Association for the Advancement of Science, Washington, DC, 2003; Chairman, Gordon Research Conference on Physical Organic Chemistry, 2003.

RESEARCH INTERESTS

The design, synthesis and study of novel organic compounds constitute the primary research activities of students and postdocs in the Scott laboratories. Our target molecules are typically chosen for their capacity to exhibit unusual molecular properties and/or abnormal chemical behavior as a consequence of unusual structural features. Uncovering and defining fundamental relationships between the structures of molecules and their properties lies at the very root of chemistry

as a science and provides the ultimate motivations for this research.

Rational laboratory syntheses of closed geodesic polyarenes (e.g., C60, higher fullerenes and their endohedral complexes) and of their open cousins (e.g., molecular bowls, baskets, belts, and tubes) currently represent many of our main objectives. Imposing curvature onto networks of trigonal carbon atoms that strive to remain planar poses a serious challenge in these syntheses, and much of our success has depended on our ability to invent and develop new synthetic methods and strategies to solve this critical problem.

Mechanism studies and the elucidation of new reaction pathways available to organic molecules at elevated temperatures also occupy much of our attention. We predicted and subsequently demonstrated, for example, the thermal scrambling of carbon atoms in benzene, naphthalene and higher polycyclic aromatic hydrocarbons, using ^{13}C isotopic labeling to reveal these otherwise invisible molecular processes. The first cases of hydrogen atom 1,2-, 1,3-, 1,4-, and 1,5- shifts in aryl radicals were likewise discovered in our lab, and a variety of unprecedented skeletal molecular rearrangements continue to engage us in this aspect of physical organic chemistry. Molecular modeling and high-level electronic structure calculations play a key role throughout all of our research.

SELECTED PUBLICATIONS

- "Synthesis of Geodesic Polyarenes by Flash Vacuum Pyrolysis," Tsefrikas, V. M.; Scott, L. T. *Chem. Reviews* 2006, 106, 4868 - 4884.
- "A Rational Chemical Synthesis of C_{60}," Scott, L. T.; Boorum, M. M.; McMahon, B. J.; Hagen, S.; Mack, J.; Blank, J.; Wegner, H.; de Meijere, A. *Science* 2002, 295, 1500-1503.
- "Methods for the Chemical Synthesis of Fullerenes," Scott, L. T. Angew. *Chem. Int. Ed.* 2004, 43, 4995-5007.

MARC L. SNAPPER, PROFESSOR

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National Science Foundation CAREER Award, 1997; Eli Lilly Grantee, 1997; Camille Dreyfus Teacher-Scholar Award, 1998; Alfred P. Sloan Research Fellowship, 1998; Glaxo Wellcome Chemistry Scholar Award, 1999.

RESEARCH INTERESTS

The interrelated aspects of our research program include introducing new chemical transformations, building complex molecules with these new reactions, and using these compounds to study cellular function.

The development of new reactions continues to be an important endeavor in organic chemistry. Our efforts have been directed toward discovering better ways of constructing medium-ring-containing compounds. Using novel transformations that build molecular complexity rapidly have allowed for the efficient construction of seven- and eight-membered ring, containing natural products. Moreover, we have also investigated whether there are new ways to discover new reactions. In this regard, we have found that "rational selection" protocols using combinatorial techniques can provide very attractive catalytic solutions to longstanding chemical problems.

Employing new reactions in the total synthesis of challenging molecules is not only important for organic chemistry; it also allows us to contribute to biological chemistry. Building molecules with unique or unusual biological activities can offer powerful new tools for studying biological systems. For example, we have used the synthesis of ilimaquinone, a marine sponge metabolite, to uncover previously unknown functional aspects of the Golgi apparatus. Similarly, other natural products currently under study will be used to provide a better understanding of the biological systems they influence.

Combining organic chemistry with select techniques in protein chemistry and molecular and cellular biology yields a powerful multidisciplinary approach for advancing our understanding of various important scientific issues.

SELECTED PUBLICATIONS

- "Catalytic Enantioselective Hosomi-Sakurai Conjugate Allylation of Acvtivated Cyclic Enones" Shizuka, M.; Snapper, M.L., *Angew. Chem. Int. Ed.* 2008, 47, 5049.
- "Intramolecular Cyclobutadiene Cycloaddition/Cyclopropanation/Thermal Rearrangement: An Effective Strategy for the Asymmetric Syntheses of Pleocarpenene and Pleocarpenone" Williams, M.J.; Deak, H.L.; Snapper, M.L. *J. Am. Chem. Soc.* 2007, 129, 486.
- "Conformationally Restricted (+)-Cacospongionolide B Analogs. Influence on Secretory Phospholipase A2 Inhibition" Murelli, R.; Cheung, A.K.; Snapper, M.L. *J. Org. Chem.* 2007, 72, 1545.
- "Enantioselective Silyl Protection of Alcohols Catalyzed by an Easily Available Amino Acid-Based Small-Molecule" Zhao, Y.; Rodrigo, J.; Hoveyda, A. H.; Snapper, M.L. *Nature* 2006, 443, 67.

KIAN L. TAN, ASSISTANT PROFESSOR

Ph.D., University of California, Berkeley, 1999-2004; NIH Postdoctoral Fellow, Harvard University, 2004-2006

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Bristol-Meyers Squibb Fellowship, 2001; American Chemical Society-Division of Organic Chemistry Fellowship, 2002; Ruth L. Kirschstein National Research Service Award, 2004.

RESEARCH INTERESTS

Our research group focuses on the development and mechanistic study of transition metal-catalyzed reactions for the formation of new carbon-carbon and carbon-heteroatom bonds. We are particularly interested in using the unique reactivity of late transition metals to engineer reactions for new and selective bond construction.

A critical challenge for synthetic chemists is control of the regio-, diastereo-, and enantioselectivity of organic transformations. Our group is currently developing a general strategy for controlling these elements through the use of an exchangeable directing group. Though we aim to develop methods that are broadly

applicable, a specific preliminary goal is the design of directing groups that allow for unusual modes of reactivity in the metal-catalyzed functionalization of olefins. To us, the ideal directing group is one that binds reversibly to organic substrates, so that it can be employed in catalytic quantities and obviate the additional steps needed for its incorporation or removal. Both exciting and challenging, the key is to identify ligand constructs that undergo rapid exchange with both the starting material and product functional groups, yet at the same time promote high efficiency and longevity for a given catalyst.

SELECTED PUBLICATIONS

- Lightburn, T.E.; Dombrowski, M.T.; Tan, K.L. "Catalytic Scaffolding Ligands: An Efficient Strategy for Directing Reactions" *J. Am. Chem. Soc.* 2008, 130, 9210-9211.
- Tan K. L.; Jacobsen E. N. "Indium-Mediated Asymmetric Allylation of Acylhydrazones Using a Chiral Urea Catalyst," Angew. *Chem. Int. Ed.* 2007, 46, 1315-1317.
- Tan, K.L.; Park S.; Ellman, J.A.; Bergman, R.G. "Intermolecular Coupling of Alkenes to Heterocycles via C-H Bond Activation." *J. Org. Chem.* 2004, 69, 7329-7335.

DUNWEI WANG, ASSISTANT PROFESSOR

Ph.D., Stanford University, 2005; Postdoctoral Fellow, California Institute of Technology, 2005-2007.

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RESEARCH INTERESTS

The research in our lab bridges the conventional disciplines of chemistry (in material synthesis), physics (property characterizations) and engineering (device constructions). We strive to tackle the daunting challenge of efficient solar energy conversion and utilization with novel nanoscale materials. Equipped with state-of-the-art facilities, we synthesize and study materials by design. Our syntheses are guided by the principles to address usually correlated material aspects one at a time. We focus our attention to the surface and interface of nanoscale structures. Our understanding will lead to products suitable for solar cell and solar fuel applications.

SELECTED PUBLICATIONS

- "TiO2/TiSi2 Heterostructures for High-Efficiency Photoelectrochemical H2O Splitting" Lin, Y.; Zhou, S.; Liu, X.; Sheehan, S.; Wang, D. *J. Am. Chem. Soc.*, 2009, 131, 2772.
- "Spontaneous Growth of Highly Conductive Two-dimensional Single Crystalline TiSi2 Nanonets" Zhou, S.; Liu, X.; Lin, Y.; Wang, D. Angew. *Chem. Int. Ed.*, 2008, 47, 7681.
- "Influence of Pressure on Si Nanowire Growth Kinetics" Zhao, H.; Zhou, S.; Hasanali, Z.; Wang, D. *J. Phys. Chem.* C, 2008, 112, 5695.

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