Department of Chemistry

In the 2005–2006 academic year, the Department of Chemistry continued its strong programs in undergraduate and graduate education. Currently there are 245 graduate students, 93 postdoctoral researchers, and 92 undergraduate chemistry majors. As of July 1, 2006, the Department faculty will comprise 32 full-time faculty members including 5 assistant, 4 associate, and 23 full professors, one an Institute Professor. In the fall, Professor Joseph P. Sadighi was promoted to associate professor without tenure, effective July 1, 2006; in the spring, Professor Timothy F. Jamison was promoted to associate professor with tenure, also effective July 1, 2006. In September 2005, Professor Arup K. Chakraborty took up a joint senior appointment as the Robert T. Haslam professor of chemical engineering, professor of chemistry, and professor of biological engineering. Professor Chakraborty obtained his PhD in chemical engineering at the University of Delaware. He came to MIT from the University of California at Berkeley, where he served as the Warren and Katherine Schlinger distinguished professor and chair of chemical engineering, and professor of chemistry from 2001 to 2005.

Highlights

The Department of Chemistry had a wonderful year. On October 2, 2005, we learned that Professor Richard R. Schrock, Frederick G. Keyes professor of chemistry, had won the 2005 Nobel Prize in chemistry for the development of a chemical reaction now used daily in the chemical industry for the efficient and more environmentally friendly production of important pharmaceuticals, fuels, synthetic fibers, and many other products. Schrock shared the prize with Yves Chauvin of the Institut Français du Pétrole and Robert H. Grubbs of Caltech "for the development of the metathesis method in organic synthesis."

Professor Richard R. Schrock speaking at a press conference at MIT on October 5, 2005. Photo: Donna Coveney

More good news followed on November 14, 2005 with the announcement from the White House that Professor Stephen J. Lippard, Arthur Amos Noyes professor of chemistry, had received the National Medal of Science for his pioneering research in bioinorganic chemistry, including the interaction of metal compounds with DNA, preparation of synthetic models for metalloproteins, and structural and mechanistic studies of methane monooxygenase.

President George W. Bush presents Professor Stephen J. Lippard with the National Medal of Science at the White House on February 13, 2006. Photo: Eric Draper, White House

The third piece of good news making the headlines came when *U.S. News & World Report* ranked MIT's Department of Chemistry number 1 in its report on the rankings of disciplines at universities around the United States.

Other Major Faculty Awards and Honors for the 2006 Academic Year

Professor Stephen L. Buchwald	2006 American Chemical Society Award for Creative Work in Synthetic Organic Chemistry
Professor Rick L. Danheiser	School of Science Dean's Educational and Student Advising Award
Professor Alan Davison	2006 Wallace H. Carothers Award for Outstanding Contributions and Advances in Industrial Applications of Chemistry 2006 American Chemical Society Award for Creative Invention
Professor Catherine L. Drennan	Named a Howard Hughes Medical Institute Professor
Professor Gregory C. Fu	2006 Mukaiyama Award
Professor Barbara Imperiali	2006 American Chemical Society Ronald Breslow Award for Achievement in Biomimetic Chemistry 2006 Emil Thomas Kaiser Award 2006 American Peptide Society Vincent du Vigneaud Award
Professor Richard R. Schrock	2006 Richards Medal of the Northeastern Section of the American Chemical Society 2006 American Chemical Society F. Albert Cotton Award in Synthetic Inorganic Chemistry
Professor Timothy M. Swager	Elected to the American Academy of Arts and Sciences 2005 Homeland Security Award sponsored by the Christopher Columbus Fellowship Foundation
Professor Alice Y. Ting	Camille Dreyfus Teacher-Scholar Award

Named Speakers

During fall 2005 and spring 2006, the following named speakers visited the Department:

Louis E. Brus, Columbia University, A. D. Little Lectures in Physical Chemistry, September 2005

Steven V. Ley, University of Cambridge, Wyeth Lecture, September 2005

Jonathan Ellman, University of California, Berkeley, George Büchi Lectures, February 2006

Jerrold Meinwald, Cornell University, Novartis Lecture in Organic Chemistry, March 2006

Kevan M. Shokat, University of California, San Francisco, Eli Lilly Lecture in Organic Chemistry, March 2006

Lucio Frydman, Weizmann Institute, A. D. Little Lectures in Physical Chemistry, March 2006

Michael A. Marletta, University of California, Berkeley, T. Y. Shen Lectures, April 2006

Jacqueline Barton, CALTECH, A. D. Little Lectures in Inorganic Chemistry, April 2006

Fred Wudl, University of California Los Angeles, Merck-Karl Pfister Lectures in Organic Chemistry, April 2006

Michael A. Abrams and John E. Ellis, inaugural Davison Symposium, May 2006

Carl P. Decicco, Bristol-Myers Squibb, and David B. Collum, Cornell University, Bristol-Myers Squibb Lectures in Organic Chemistry, May 2006

Dr. T. Y. Shen and Professor Michael A. Marletta, Aldo DeBenedictis distinguished professor of chemistry at the University of California, Berkeley, who delivered the T. Y. Shen Lectures in Biological Chemistry in April.

Education

In this past academic year, Sylvia Ceyer began her tenure as the associate department head in charge of the academic program. In this capacity, she serves as the academic officer, representing the department at the Institute level on all academic issues. Sylvia replaced Rick Danheiser, who had served in this role for the last 10 years. On the horizon, Sylvia will oversee a revamping of the undergraduate laboratory curriculum, dubbed URIECA, which is short for undergraduate research-inspired experimental chemistry alternatives. URIECA will replace the 5.311, 5.32, 5.33 sequence with a series of modules integrating faculty research with undergraduate learning. Greater flexibility in student workload and scheduling, opportunities for freshmen to take laboratory subjects, and the fostering of interactions between undergraduates, graduates, postdocs, and faculty are major goals for the new curriculum. A few of the new URIECA experiments will be introduced into the existing laboratory format this academic year before implementation of the complete URIECA sequence in fall 2007.

Last fall, the physical chemistry faculty and the faculty of the new biological engineering division launched an initiative to co-teach the basics of thermodynamics. The two classes, 5.60J and 20.110J (BE), were co-taught with great success by faculty from both departments. Moungi Bawendi taught thermodynamics, with a smattering of statistical concepts, during the first half of the semester to both 5.60 and BE.110 students. At mid-semester, the two classes split, and the 5.60 chemistry students began learning advanced thermodynamics and kinetics concepts with Robert Field, while the 20.110 students received instruction in introductory biological engineering concepts from Biological Engineering faculty.

In fall 2006, 45 students will enter the graduate program of the Chemistry Department; from September 2005 through June 2006, the department awarded 45 PhD degrees and 3 MS degrees. In undergraduate education, 28 students graduated in June with BS degrees in chemistry. The 2005 Undergraduate Spring Awards Banquet was held on Thursday, May 18, in the MIT Museum. The following awards were presented:

Alpha Chi Sigma Award	Sarah Mahlstedt
Research Award	Rachel E. Tundel Stephen J. Fredette Timothy C. Davenport
Frederick D. Greene Teaching Award	Stephen J. Fredette Shan Riku Jessica L. Hagelstein
Merck Index Award	Stephen J. Fredette Maryann E. Racine
Hypercube Scholar Award	Surasak Chunsrivirot

American Institute of Chemists Foundation Award	Timothy C. Davenport
ACS Analytical Chemistry Award	Mandeep K. Virdi Eric A. McNeill
CRC Press Freshman Chemistry Achievement Award	Hyun (Tony) Kim
Association of MIT Alumnae (AMITA) Senior Academic Award	Sarah Mahlstedt

Seniors (L–R): Surasak Chunsrivirot, Rachel Tundel, Kate Stafford, Prathima Nandivada, Jacqueline Tio, Maryann Racine (back), Yuri Matsumoto, Sarah Mahlstedt, Emily Fenn, Evans Boney (back), Josh Katz, Tulasi Khandan, Cindy Yuan, Daniel Nedelcu, Lara Collazo, Stephen Fredette, Timothy Davenport.

Graduate Student Awards and Honors

Ryan Altman, Buchwald Group	Pfizer Fellowship
Julien Bachmann, Nocera Group	Alexander von Humboldt Fellowship (from Germany)
Peter Bernhardt, O'Connor Group	MIT Robert T. Haslam Presidential Fellowship
Julian Chan, Swager Group	MIT-DuPont Presidential Fellowship
Ziad Ganim, Tokmakoff Group	Morse travel grant
Lesley-Ann Giddings, O'Connor Group	NSF Graduate Research Fellowship Ford Foundation Diversity Predoctoral Fellowship
Evan Guggenheim, Lippard Group	International Precious Metals Institute (IPMI) Student Award
Ken Hamill, Ting Group	NSF Graduate Research Fellowship
Kirsten Johnson, Molina Group	Fellowship at Pacific Northwest National Laboratory (PNNL) in their Summer Research Institute program
Lucy Kohnen, Danheiser Group	NSF Graduate Research Fellowship Ford Foundation Diversity Fellowship (declined) Henry Bromfield Rogers Fellowship Morse travel grant David Johnson Fellowship Pfizer Research Fellowship
Maksym Kryvohuz, Cao Group	Milas Fund Fellowship
David Lahr, Ceyer Group	National Research Council (NRC) fellowship
Mi Hee Lim, Lippard Group	Martin Family Fellowship
Wan-Chen Lin, Licht Group	CSBi-Merck Predoctoral Fellow
Sam Lipoff, Field Group	NSF Graduate Research Fellowship Department of Homeland Security Graduate Fellowship
Wenhao Liu, Bawendi Group	MIT Praecis Presidential Graduate Fellowship NSF Graduate Research Fellowship
Emily McLaurin, Nocera Group	Corning Fellowship

Elizabeth McCoy, O'Connor Group	Novartis Graduate Fellowship in Organic Chemistry for Minorities and Women
Jong-Ho Park, Molina Group	Kwanjeong Fellowship, August 2005
Laura Phillips, Drennan Group	Martin Fellow for Sustainability Cambridge Science Foundation Travel Grant Accepted to Biotechnology Training Program
Peter Rye, Essigmann Group	Karl Taylor Compton Prize The Compton Prizes are given in memory of Dr. Karl Taylor Compton, president of the Institute from 1930 to 1949 and chairman of the Corporation from 1949 to 1954. They are the highest awards presented by the Institute to students and student organizations in recognition of excellent achievements in citizenship and devotion to the welfare of MIT. They reflect outstanding contributions to the MIT community as a whole, sustained over a significant number of years.
Sarah Slavoff, Ting Group	Whitaker Health Sciences Fund Fellowship
Zachary J. Tonzetich, Schrock Group	Alan Davison Fellow
Jessica Vey, Drennan Group	Ludo Frevel Crystallography Fellowship from the International Union of Crystallography

Research Highlights

Moungi G. Bawendi
Professor Bawendi's research group has continued progress in the synthesis of new nanocrystal quantum dots, the spectroscopy of quantum dots, devices incorporating quantum dots, and biomedical applications of quantum dots. His students have demonstrated new quantum dot heterostructures with potential applications in photovoltaics and biomedical imaging. They are investigating potential evidence of carrier multiplication in quantum dots, an effect that could be important in improving the quantum efficiency of photovoltaic devices. They, in collaboration with Professors Vladimir Bulovic and Marc Kastner have demonstrated novel photoconductive and light-emitting devices based on quantum dots. Bawendi's students, with collaborators at Massachusetts General Hospital and Beth Israel Deaconess Medical Center, have investigated in vivo imaging applications of quantum dots, with one project in particular concentrating on demonstrating renal clearance in animal models.

Stephen L. Buchwald
Professor Buchwald's work during the past year has focused on developing methods that are of use in both academia and industry. In particular, his work on metal-catalyzed methods for carbon-nitrogen bond formation are among the most important to the pharmaceutical industry and are used on a daily basis in essentially all major companies.

Arup Chakraborty
The central theme of Arup Chakraborty's research is to develop and apply statistical

mechanical methods that can fruitfully complement genetic, biochemical, and imaging experiments (carried out by collaborators) to discover the principles that govern the adaptive immune response to pathogens. Chakraborty's recent work has helped elucidate how T lymphocytes detect minute amounts of antigen-derived peptide-major histocompatibility complex (MHC) molecules without frequent spurious triggering due to endogenous peptide-MHC molecules displayed on antigen-presenting cells. His efforts to bring together statistical physics and T cell biology have led to establishment of the Immune Response Consortium, a center funded by the National Institutes of Health (NIH) (MIT is the lead institution and Chakraborty is the principal investigator), which has brought together leading immunologists, physical scientists, and engineers to develop principles and predictive models of T lymphocyte activation.

Christopher C. Cummins
In the past year, the Cummins laboratory has focused on the achievement and description of synthetic cycles for the synthesis of organonitrogen and organophosphorus compounds starting from the elemental molecules N_2 and P_4. The latter small molecules are abundant primary sources of the zerovalent elements nitrogen and phosphorus, both of which are crucial to life. The work seeks to overcome chemical challenges associated with utilization of these elemental molecules. A second research theme, being pursued collaboratively, is the discovery of new O-O bond-forming reactions relevant to solar energy.

Rick L. Danheiser
Highlights of research accomplished in the Danheiser laboratory in 2005 include the completion of a very efficient total synthesis of the neurotoxic alkaloid quinolizidine (–)-217A and the development of methods for synthesizing several important ring systems, including indoles and highly substituted cyclopentenones. In the area of green chemistry, a strategy was developed for synthesizing nitrogen-containing compounds in environmentally friendly media, such as supercritical carbon dioxide.

Catherine L. Drennan
In the March 16, 2006, issue of *Nature*, the Drennan group reported the first crystal structure of an iron-dependent halogenase. This structural analysis reveals a novel coordination environment for the catalytic iron and suggests a mechanism by which nature can harness the catalytic prowess necessary to perform the most chemically challenging of halogenation reactions. This work provides an important step forward in understanding the biological synthesis of medically useful halogenated natural products such as antibiotics and antitumor agents.

Gregory C. Fu
During the past year, the Fu group has developed a variety of carbon-carbon bond-forming processes, catalyzed by nickel, that are of potential interest to a wide array of scientists, including chemists, biologists, and material scientists. In addition, they have described a series of catalytic asymmetric reactions (O-H insertions, cycloadditions, processes that generate b-lactams).

Barbara Imperiali
Professor Imperiali's research targets the development of innovative chemical tools for studying complex biological systems. In particular, methods for sensing kinase activities and generating caged phosphopeptides and proteins are being developed for studies of cell migration, cell cycle control, and regulation of synaptic plasticity. Also, major progress has been made in applying lanthanide-binding tags, discovered in the group, in

structural and functional proteomics. Research on the comparative analysis of eukaryotic and prokaryotic protein glycosylation continues to be very exciting.

Timothy F. Jamison
The theme of Jamison's research is the discovery and implementation of new reactions for organic synthesis. Many of the targeted transformations are based on common structural motifs or functional group patterns present in molecules provided by Nature, while others have their origins in unexpected products obtained in the course of other experiments. In the past year, Jamison's group developed several such chemical reactions, and they have made it possible to synthesize several complex molecules that may lead to new treatments for a variety of diseases, including cancer and AIDS.

Alexander Klibanov
Current research interests in the Klibanov group are in the following areas: enzymatic catalysis in nonaqueous solvents, enzymes as stereoselective catalysts in organic synthesis, novel microbicidal materials, and stabilization and delivery of macromolecular pharmaceuticals (DNA and proteins).

Stuart Licht
The Licht group is studying how proteins can function as molecular machines. They are investigating the coupling of chemical energy to protein conformational changes both in an ion channel that controls insulin secretion and in an enzyme that unfolds protein substrates and cleaves them into small fragments. They are also developing chemical tools to fine-tune ion channel kinetics with the goal of controlling the kinetics of synaptic currents.

Stephen J. Lippard
A Cu(II) fluorescein construct was prepared that reacts with nitric oxide to produce a bright fluorescent signal, affording the first turn-on sensor for direct detection of NO in living cells. A platinum anticancer drug cross-link on the nucleosome dictates the rotational setting of the DNA with respect to the core histones. A peroxo diiron(III) intermediate was identified in the reaction of reduced toluene/*o*-xylene monooxygenase with O_2. Novel diiron(II) models for the active site of this and related enzymes were reported that react with O_2 and oxidize substrates.

Mohammad Movassaghi
Professor Movassaghi's research program continues to focus on developing strategies and technologies relying on a cascade bond-forming reaction for complex molecule synthesis. His group has completed the first total synthesis of optically active galbulimima alkaloids, revised their previously assigned absolute stereochemistry, and developed synthetic methodologies based on their original hypothesis on their biogenesis. They have completed a concise synthesis of (–)-irofulven, a compound in a phase II clinical trial for treatment of a number of cancers, and devised a unifying strategy to access the bioactive core of this family of compounds. They have continued to develop new and practical methodologies for the rapid synthesis of important azaheterocycles that are ubiquitous in natural products, pharmaceuticals, and functional materials.

Keith A. Nelson
Keith Nelson's research in ultrafast dynamics of complex condensed matter and advanced materials yielded unique results, including the first direct, real-time observations of irreversible chemical reactions in organic crystals, where the regularity of the crystal lattice structure permits detailed modeling of the pathways followed by each molecular fragment. The results will be published in *Science*. Ultrafast phase transitions in crystalline solids also were observed. In separate work, high-intensity terahertz waves were generated and used to drive nonlinear lattice responses and to probe the dynamics of structural phase transitions in ferroelectric crystals. Current work is aimed at even stronger terahertz fields that can be used for extensive control over macroscopic material structure, with dynamically induced structural changes monitored directly in real time.

Sarah E. O'Connor
Understanding the enzymes that catalyze natural product biosynthesis allows reprogramming of biosynthetic pathways to produce novel molecules with improved pharmacologic activities. O'Connor's research has shown that periwinkle can be used to produce a diverse array of natural product analogues. Additionally, the central enzyme of this pathway has been redesigned to selectively accept nonnatural substrates. The use of plant biosynthetic pathways to generate novel compounds is largely unprecedented because of the greater chemical, genetic, and developmental complexity of higher eukaryotic metabolic pathways.

Richard R. Schrock
Professor Schrock's research is in the area of high-oxidation-state early metal organometallic chemistry and is sponsored by the National Science Foundation and NIH. He is also sponsored by the Army and the Department of Energy in the area of controlled polymer synthesis. Finally, NIH also supports a project concerned with reducing molecular nitrogen at room temperature and pressure.

Robert J. Silbey
During the past year, Professor Silbey continued his research in theoretical chemistry, studying single molecule spectroscopy, proton-coupled electron transfer, and energy transfer in light-harvesting complexes. In the latter study, he and his graduate student Y. C. Cheng showed that a small amount of coherent interactions in the B800 band in LH2 markedly changes the spectrum and energy transfer rates.

JoAnne Stubbe
Ribonucleotide reductases (RNRs) catalyze an essential step in DNA replication and repair by converting nucleotides to deoxynucleotides. Their central role in nucleic acid metabolism has made them the successful target of two drugs used clinically to treat cancer. One of these drugs, Gemzar, was designed based on the mechanism of reduction Stubbe's group unraveled over the past two decades. They are studying the detailed mechanism of RNR inactivation by phosphorylated Gemzar and have made excellent progress this past year. The second drug has long been thought to reduce and inactivate the essential tyrosyl radical of RNR. Their studies on the unusual mechanism of radical propagation suggest that this is not the case. The studies on these compounds will provide insight into the design of more potent therapeutics.

Timothy M. Swager
Timothy M. Swager's group has developed a number of new polymer and liquid crystal concepts. New polymers with high ionization potential were developed and these materials are potentially useful in creating all polymer photovoltaic devices. A collaborative effort between Edwin L. Thomas (Department of Materials Science and Engineering) and Swager has resulted in demonstration of a new method for creating polymers with improved ductility and strength. The latter methods have many promising applications in materials for ballistic and blast protection.

Alice Ting
In the past year, Alice Ting's research group has developed and improved several methodologies for cellular imaging of protein function. These include a new protein interaction detection method based on biotin ligase, site-specific protein labeling in cells using lipoic acid ligase, single molecule imaging of receptor trafficking using monovalent quantum dots, and multicolor labeling in cells using an engineered biotin ligase-peptide substrate orthogonal pair.

Andrei Tokmakoff
The Tokmakoff group is advancing experimental methods to study molecular dynamics in solution. Their primary tool is two-dimensional infrared spectroscopy—a transient probe of molecular structure. During the past year, they have revealed mechanisms of hydrogen-bonding rearrangements in water, probed the folding mechanisms of proteins and peptides, and developed methods to directly compare their experiments with molecular dynamics simulations.

Troy Van Voorhis
The Van Voorhis group has made significant advances in describing electron transfer reactions using first principles of electronic structure techniques. They have developed density functional-based methods for describing the dynamics and energetics of electron motion. Their work has the potential to greatly affect the describing and designing of novel functional electronic materials.

Timothy M. Swager
Department Head
John D. MacArthur Professor of Chemistry

More information about the Department of Chemistry can be found at http://web.mit.edu/chemistry/www/.