

## Department of Chemistry

In the 2007–2008 academic year, the Chemistry Department continued its strong programs in undergraduate and graduate education. Currently, there are 245 graduate students, 103 postdoctoral researchers, and 81 undergraduate chemistry majors. As of July 1, 2008, the Chemistry Department faculty will comprise 31 full-time faculty members, including one assistant, four associate, and 23 full professors, two of whom are Institute Professors. Catherine Drennan was promoted to full professor, and Mohammad Movassaghi, Sarah O'Connor, and Troy Van Voorhis were promoted to associate professor without tenure. All of these promotions will take effect on July 1, 2008.

### Highlights

#### **Buchwald and Swager Elected to the National Academy of Sciences**

Professors Stephen L. Buchwald and Timothy M. Swager have been elected to the National Academy of Sciences (NAS) in recognition of their distinguished and continuing achievements in original research. Election to NAS, a private organization of scientists and engineers dedicated to advancing science and its use for the general welfare, is considered a top honor for those in the science and engineering fields. Established in 1863, NAS acts as an official advisor to the federal government, upon request, in any matter of science or technology. Faculty members previously elected include Professors Robert A. Alberty, Mounqi G. Bawendi, Klaus Biemann, Sylvia T. Ceyer, H. Gobind Khorana, Alexander M. Klibanov, Stephen J. Lippard, Richard R. Schrock, Dietmar Seyferth, Robert J. Silbey, JoAnne Stubbe, John S. Waugh, and Gerald N. Wogan.

#### **Drennan Selected as Howard Hughes Medical Institute Investigator**

In May 2008, Catherine L. Drennan, professor of chemistry and biology and Howard Hughes Medical Institute (HHMI) professor, was selected as an HHMI investigator. HHMI investigators continue to push the bounds of knowledge in many of the hottest areas in biomedical research. Widely recognized for their creativity and productivity, the current group of HHMI investigators includes 12 Nobel Prize winners and 122 members of the National Academy of Sciences. Professor Drennan is the first HHMI professor ever to be named an HHMI investigator, bringing the total number of current MIT professors holding the distinction to 19.

#### **Cummins Elected to the Academy of Arts and Science**

Professor Christopher C. Cummins has been elected to the American Academy of Arts and Sciences. The Academy, one of the nation's oldest and most prestigious honorary societies and independent policy research centers, announced on April 28, 2008 the election of a new class of members. "The Academy honors excellence by electing to membership remarkable men and women who have made preeminent contributions to their fields, and to the world," said Academy president Emilio Bizzi. Professor Cummins joins a distinguished group of current and emeritus faculty members who are fellows of the Academy, namely, Robert A. Alberty, Mounqi G. Bawendi, Klaus Biemann, Stephen L. Buchwald, Sylvia T. Ceyer, Arup K. Chakraborty, John M. Deutch, Robert W. Field,

Gregory C. Fu, Frederick D. Greene, Barbara Imperiali, H. Gobind Khorana, Stephen J. Lippard, Daniel G. Nocera, Irwin Oppenheim, Richard R. Schrock, Dietmar Seyferth, Robert J. Silbey, and JoAnne Stubbe.

### **Nocera to Direct the Solar Revolution Project**

Professor Daniel G. Nocera was chosen to direct the Solar Revolution Project (SRP). Funded by a \$10 million gift from the Chesonis Family Foundation, SRP will explore new materials and systems that could dramatically accelerate the availability of solar energy. SRP will complement and interact closely with other large solar projects at MIT, creating one of the largest solar energy clusters at any research university.

The Chesonis gift will allow MIT to explore bold approaches that are essential for transforming the solar industry. Specifically, it will focus on three elements—capture, conversion, and storage—that will ultimately make solar power a viable, near-term energy source.

*[Launching a solar revolution: MIT gets \$10M gift from Chesonis Family Foundation to advance solar technologies, MIT Tech Talk 2008 52(24):8.]*

### **Other Major Faculty Awards and Honors for the 2008 Academic Year**

Stephen L. Buchwald, Camille Dreyfus professor of chemistry—Elected to the National Academy of Sciences

Sylvia T. Ceyer, John C. Sheehan professor of chemistry—2008 Arthur C. Smith Award

Christopher C. Cummins, professor of chemistry—Elected to the American Academy of Arts and Sciences

Catherine L. Drennan, professor of chemistry and biology, HHMI professor—Promoted to full professor, awarded an MIT Energy Initiative Seed Grant for Energy Research, selected as a Howard Hughes Medical Institute Investigator

Gregory C. Fu, Firmenich professor of chemistry—Appointed Firmenich professor of chemistry

Daniel S. Kemp, professor emeritus—Roche-Meienhofer Award for Peptide Science

Alexander M. Klibanov, Novartis professor of chemistry and bioengineering—Appointed Novartis professor of chemistry and bioengineering

Stephen J. Lippard, Arthur Amos Noyes professor of chemistry—2008 International Precious Metals Institute Student Advisor Award

Mohammad Movassaghi, associate professor of chemistry—2008 Camille Dreyfus Teacher-Scholar Award, 2008 Alfred P. Sloan Fellowship, 2007 Eli Lilly Grant in Organic Chemistry, MIT Energy Initiative Seed Grant for Energy Research

Daniel G. Nocera, Henry Dreyfus professor of energy and professor of chemistry—Appointed director of the Solar Revolution Project, elected fellow of the American Association of the Advancement of Science, received the 2008 Harrison Howe Award from the Rochester Section of the American Chemical Society

Richard R. Schrock, Frederick G. Keyes professor of chemistry—Elected to the Royal Society (London), conferred an honorary degree by the University of Zaragoza, Spain

JoAnne Stubbe, Novartis professor of chemistry and professor of biology—2008 John Gamble Kirkwood Medal, National Academy of Sciences Award in Chemical Sciences, 2008 Emil Kaiser Award

Timothy M. Swager, John D. MacArthur professor of chemistry, head of the department—Elected to the National Academy of Sciences, conferred an honorary degree of science by the University of Montana

Steven R. Tannenbaum, Underwood-Prescott professor of toxicology and chemistry—2008 American Association for Cancer Research Award for Outstanding Achievement in Chemistry in Cancer Research

Alice Y. Ting, associate professor of chemistry—American Chemical Society (Eastern New York Section) 2007 Buck-Whitney Award

Troy Van Voorhis, associate professor of chemistry—MIT Energy Initiative Seed Grant for Energy Research

### **Named Lectures**

During fall 2007 and spring 2008, the Department welcomed many speakers who gave named lectures:

Michael Graetzel, Institute of Physical Chemistry, École Polytechnique Fédéral de Lausanne—A.D. Little Lectures in Inorganic Chemistry

Carlos Bustamante, University of California, Berkeley and Howard Hughes Medical Institute—A.D. Little Lectures in Physical Chemistry

Jun Terao, Osaka University—Merck-Banyu Lecture in Organic Chemistry

Robert H. Grubbs, California Institute of Technology—Wyeth Lecture in Organic Chemistry

William Fenical, Scripps Institute of Oceanography and University of California, San Diego—George Buchi Lectures in Organic Chemistry

Peter Walter, University of California, San Francisco—T.Y. Shen Lectures

Jon Thorson, University of Wisconsin and Nicholas Meanwell, Bristol-Myers Squibb—Bristol-Myers Squibb Lectures in Organic Synthesis

Scott Denmark, University of Illinois, Urbana-Champaign and Adrian D. Hobson, Abbott Bioresearch Center—Abbott Lecture in Organic Chemistry

Anna Mapp, University of Michigan—Eli Lilly Lecture in Organic Chemistry

Harry L. Anderson, University of Oxford—Merck-Karl Pfister Lectures in Organic Chemistry

M. Frederick Hawthorne, University of Missouri–Columbia—Davison Lecture in Inorganic Chemistry

Erik Sorensen, Princeton University—Boehringer Ingelheim Lecture in Organic Chemistry



*Peter Walter, Sarah O'Connor, and T. Y. Shen*

## **Undergraduate Education**

In the area of undergraduate education, 31 students graduated in 2008 with SB degrees in chemistry. The 2008 Undergraduate Senior Recognition and Awards Banquet was held on Thursday, May 15, at the R&D Common Era in the Stata Center. The following awards were presented:

Alpha Chi Sigma Award for distinguished scholastic achievement, originality, and breadth of interest in chemistry—Chawita Netirojjanakul, Emily Y. Tsui

Research Award for outstanding contributions in the area of research—Ziliang Lin, Brian A. Sparling

Service Award for significant contributions in the area of service to the department—Jiho Lee

Frederick D. Greene Teaching Award—Brian A. Sparling, George S. Zaidan

Merck Index Award for outstanding scholarship—Pareesh Agarwal, Ziliang Lin, Rishi Venkata Puram, George S. Zaidan

Hypercube Scholar Award in recognition of outstanding contribution to the advancement of computational chemistry—George S. Zaidan

Strem Award, in recognition of the best undergraduate research presentation at the UROP Symposium on April 26, 2008—Mihai Dudata

American Chemical Society Analytical Chemistry Award for an outstanding analytical chemist (junior year)—Veena Venkatachalam

Sophomore Achievement Award for outstanding performance in academics, research, and service to the department—Michael R. Blaisse, Sid E. Creutz, Fan Liu

CRC Press Freshman Chemistry Achievement Award for outstanding academic achievement in chemistry—Patricia A. Widener

Barry M. Goldwater Award for Excellence in Education—Annelise R. Beck (junior)

### **Undergraduate Education**

Course 5 majors display incredible enthusiasm for chemistry and for this department. Whether it was being the guinea pigs of a new lab curriculum or responding to the myriad requests for majors to “chat up” Course 5, our students turned out ready for action. They are an incredible, inspiring group of young people.

This kind of dedication to the craft, however, does not just happen. It requires the patience and caring of strong mentors, namely our faculty, postdocs, and graduate students. They are incredibly diligent in providing the very best learning environment for our students. Whether it is in the classroom, in the research lab or in some other advising role, they offer a fertile ground upon which the next generation of scientists can learn and grow.

### **URIECA Roll Out**

Under the direction of Dr. Mariusz Twardowski, AY2008 saw the launch of the new Undergraduate Research-Inspired Experimental Chemistry Alternatives (URIECA) lab curriculum. It began in the fall with the first four teaching modules, with two more added in the spring. Chemistry majors are delighted with the new sequence and realize that they are on the cutting edge of a new way of teaching—and learning—chemistry. Roll out of phase 2 of the new curriculum will begin in fall 2008. By the end AY2009, the all 12 modules of the URIECA curriculum will be operational.

### **Expanded Tutoring Program**

During the past several years, we have only offered one-on-one tutoring to students enrolled in 5.111/5.112 Principles of Chemical Science. This year, we expanded our tutoring program to include all the required undergraduate chemistry classes. With subject tutoring teams of both graduate and undergraduate students, we offered one-on-one tutoring to 130 students over the fall and spring terms. This new program has been well received by our students. One student wrote: “...I know I would not have passed without the extra explanations and encouragement.” Another student wrote: “It really helped me...It would be great if you pressured [another] department to provide the same type of accessible and personable tutors! Thank you so much.”



### New Teaching Assistant Training Program

Reflecting back on previous teaching assistant (TA) training programs the department has offered over the years, we concluded that trying to pack everything into two days was a bit like forcing our new TA's "to drink from that proverbial fire hose." With the guidance and leadership of Dr. Sanjoy Mahajan of the MIT Teaching and Learning Lab, we developed a new training program that now consists of four half-day sessions and includes new seminars on teaching the art of problem solving, interactive learning, and lesson planning. These new sessions all lead toward the "microteaching" session, at which TAs have the opportunity to teach, be videotaped, and receive feedback before meeting their classes for the first time. Although Chemistry TAs generally receive very high ratings on their teaching evaluations, we believe that this new expanded program better prepares our TAs for their work in the lab and classroom and enhances their professional development as future leaders in the field of chemistry.

### UROP Publications

The Undergraduate Research Opportunities Program (UROP) remains the capstone experience for our undergraduates. With over 90% of our majors working in a research group (the majority in chemistry), they have the unique opportunity to conduct research alongside faculty, postdocs and graduate students. In the recent senior survey, one student commented: "My UROP experience has defined my undergraduate education at MIT, and 'very satisfied' is certainly an understatement of how I feel towards the subject."

The following is a sample of recent publications with chemistry majors (in bold) as authors:

Altman RA, Shafir A, Choi A, **Lichtor, PA** and Buchwald SL. An improved Cu-based catalyst system for the reactions of alcohols with aryl halides, *Journal of Organic Chemistry* 2008, 73(1):284–286. PMID: 18044928.

Rye PT, Delaney JC, **Netirojjanakul C**, Sun DX, Liu JZ, Essigmann JM. Mismatch repair proteins collaborate with methyltransferases in the repair of O(6)-methylguanine, *DNA Repair (Amst)*. 2008, 7(2):170–176. PMID: 17951114.

**Sparling BA**, Moslin RM, Jamison TF. SmI<sub>2</sub>-promoted Reformatsky-type coupling reactions in exceptionally hindered contexts, *Organic Letters* 2008, 10(6):1291–1294. PMID: 18302397.

Hubbard PA, Padovani D, Labunska T, **Mahlstedt SA**, Banerjee R, and Drennan CL. Crystal structure and mutagenesis of the metallochaperone MeaB: insight into the causes of methylmalonic aciduria, *Journal of Biological Chemistry* 2007, 282(43):31308–31316. PMID: 17728257.

### Course 5 Events

The majors are active promoters of Course 5 and were on hand to talk with freshmen at the Academic Expo in August, the Exploring the Majors Fair in November, and the

Freshman Open House in March. They also entertained children and their parents with the Chemistry Magic Show during Family Weekend in October (one of the most popular events offered at MIT during this weekend). During Campus Preview Weekend in April, ClubChem gave tours of their UROP labs to over 60 prefreshman and their parents. (We were expecting perhaps 20!) After giving the tours, the majors invited everyone back to the lounge for refreshments and discussion. So many wished to return to hear more about Course 5 that we had to move the gathering to classroom 4-270. Chemistry majors at work!

### **Graduate Awards**

Omar Ahmad (Movassaghi Group)—Merck Summer Graduate Fellowship

Peter Allen (Bawendi Group)—Morse Travel Grant

Sarah Barkow (Sauer Group)—Morse Travel Grant, MIT Student Leadership Award

Loren Andreas (Griffin Group)—National Science Foundation Graduate Research Fellowship

Josh Baraban (Field Group)—National Science Foundation Graduate Research Fellowship, David A. Johnson Summer Graduate Fellowship

Peter Bernhardt (O'Connor Group)—Amgen Summer Fellowship

Johnathan Cheng (O'Connor Group)—DuPont-MIT Presidential Fellowship

Joseph Cotruvo (Stubbe Group)—National Defense Science and Engineering Graduate Fellowship

Shaun Fontaine (Danheiser Group)—George H. Buchi Summer Graduate Fellowship, AstraZeneca Graduate Fellowship in Organic Chemistry

Ziad Ganim (Tokmakoff Group)—Daniel S. Kemp Summer Fellowship, Poitras Predoctoral Fellowship

Meredith Hartley (Imperiali Group)—Wyeth Predoctoral Fellowship, through the American Chemical Society Division of Medicinal Chemistry

Harold Hwang (Nelson Group)—Morse Travel Grant

Alan Hyde (Buchwald Group)—Professor Nicholas A. Milas Fellowship

Numpon Insin (Bawendi Group)—Morse Travel Grant

Yan Kung (Drennan Group)—Morse Travel Grant



*Hooding Ceremony, June 2008*

Justin Kim (Movassaghi Group)—National Defense Science and Engineering Graduate (NDSEG) Fellowship, National Science Foundation Fellowship (but declined the award in favor of the NDSEG award), Presidential Graduate Fellowship

Józef Lewandowski (Griffin Group)—Marie Curie International Reintegration Grant from the European Union to study protein dynamics at the École normale supérieure, Lyon, France.

Wenhao Liu (Bawendi Group)—Morse Travel Grant

Elvedin Lukovic (Imperiali Group)—Morse Travel Grant

Kara Manke (Nelson Group)—National Science Foundation Graduate Research Fellowship

Mike Marshak (Nocera Group)—Research fellowship from the French oil company, Total

Lisa Marshall (Bawendi Group)—Morse Travel Grant



Ellen Minnihan (Stubbe Group)—C.P. Chu and Y. Lai Summer Graduate Fellowship

Steve Presse (Silbey Group)—Fonds québécois de recherche sur la nature et les technologies (FQRNT) postdoctoral fellowship

Sean Roberts (Tokmakoff Group)—Morse Travel Grant

Kristin Schleicher (Jamison Group)—Novartis Graduate Fellowship in Organic Chemistry for Minorities and Women, for AY2008

Christian Schubert (Kemp Group)—Goodwin Medal, Lewis Paul Chapin Fellowship

Daniel Seuss (Peters Group)—National Science Foundation Graduate Research Fellowship

Wenchao Sheng (ShaoHorn Group)—Morse Travel Grant

Christina Stock (Drennan Group)—National Institutes of Health Biotechnology Training Program Grant

Stefanie Sydlik (Swager Group)— National Science Foundation Graduate Research Fellowship

Meiliana Tjandra (Movassaghi Group)—Bristol-Myers Squibb Fellowship

Aaron Van Dyke (Jamison Group)—Wyeth Scholarship, Morse Travel Grant

Brett VanVeller (Swager Group)—Canadian National Science and Engineering Research Council Postgraduate Scholarship

Ivan Vilotijevic (Jamison Group)—Merck Summer Graduate Fellowship

Cintyu Wong (Drennan Group)—Morse Travel Grant

Peng Zhou (Ting Group)—Lewis Paul Chapin Fellowship

Eric Zimanyi (Silbey Group)— Fonds québécois de recherche sur la nature et les technologies (FQRNT) Doctoral Research Scholarship

## **Research Highlights**

### **Moungi G. Bawendi**

Professor Bawendi and his students have continued their studies of semiconducting and magnetic nanocrystals. They have developed new types of nanocrystals. They have collaborated with Professors Bulovic and Kastner on measuring optoelectronic properties of thin films of nanocrystals. They have collaborated with Professors Nocera and Ting on designing new nanocrystal chemistry for use in imaging of cells. They

have also collaborated with groups at Massachusetts General Hospital and Beth Israel Deaconess Medical Center to design and apply nanocrystals in biomedical (in vivo) applications.

### **Stephen L. Buchwald**

The Buchwald group has made progress in their work to develop increasingly general catalysts for carbon-carbon and carbon-heteroatom bond-forming reactions. In particular, they have prepared a new class of precatalysts that give unprecedented reactivity for these transformations. Moreover, this allows them to study a variety of mechanistic details about this chemistry.

### **Arup Chakraborty**

The Chakraborty group has made a significant advance in elucidating a long-standing problem in immunology; viz., how T cell development in the thymus results in a T cell repertoire which is both antigen-specific and cross-reactive at the same time. The resulting papers are on the verge of being accepted in *Cell* (with the Weiss lab at the University of California, San Francisco) and *Proceedings of the National Academy of Sciences*.

### **Catherine L. Drennan**

The Drennan group has continued studies of carbon monoxide dehydrogenase/acetyl-CoA synthase (CODH/ACS), publishing a structure of CODH/ACS with xenon gas in *Biochemistry* in 2008. This structure allowed the group to describe the nature of an amazing 140Å-long enzyme channel. They have also extended their work in the area of natural product biosynthesis, publishing structures of rebeccamycin and violacein biosynthetic enzymes in *Proceedings of the National Academy of Sciences* in 2007 and *Journal of Biological Chemistry* in 2008, respectively.

### **John M. Essigmann**

The Essigmann group had two significant accomplishments in AY2008. Both were follow-ups to their discovery three years ago that the DNA repair protein, AlkB, acts in vitro to repair the DNA lesions of vinyl chloride and chloroacetaldehyde, two important industrial chemicals and human carcinogens. The first study showed in a cellular system that AlkB indeed does protect cells against chloroacetaldehyde, thus verifying the importance of this repair enzyme as a defense against toxicity. The second study showed that the enzyme also is involved in suppressing the toxicity of BCNU, an important chemotherapeutic agent used against brain tumors. Thus AlkB expression would lead to tumor resistance and clinical therapy. The study identifies inhibition of AlkB as a strategy to kill brain tumors.

### **Robert W. Field**

The Field group, in collaboration with Professor Brooks Pate (University of Virginia) Dr. Kirill Kuyanov, Adam Steeves, and Barratt Park, has demonstrated the revolutionary capabilities of a chirped pulse millimeter wave spectrometer, ideally suited for characterizing the extremely large amplitude eigenstates localized along the acetylene-

vinylidene isomerization path. Dr. Wilton Virgo and Kyle Bittinger have demonstrated a new method, using time-gated fluorescence excitation spectroscopy, that provides the first complete mechanistic description of doorway-mediated intersystem crossing.

### **Gregory C. Fu**

The Fu group has developed effective nickel catalysts for useful carbon-carbon bond-forming reactions, including processes that control the chirality (handedness) of the products. In addition, they have discovered palladium catalysts that achieve interesting cyclization reactions, as well as copper catalysts.

### **Barbara Imperiali**

The Imperiali group's research continues to focus on the design, synthesis, and application of innovative chemical tools for the study of complex biological systems. In particular, methods for sensitive and selective methods for diagnosing the dynamic fluctuations of enzyme activities, such as kinases, and protein/protein interactions are being developed for studies of cell migration, cell cycle control, and the regulation of synaptic plasticity. Ongoing research also focuses on glycosylation in prokaryotes with the goal of understanding the roles of cell surface carbohydrates in infection and pathogenicity.

### **Timothy F. Jamison**

The theme of the Jamison group's research is the discovery and implementation of new reactions for organic synthesis. Many of the transformations they target assemble functional group patterns present in molecules found in nature and/or pharmaceuticals. The group is also inventing reactions that convert carbon dioxide (CO<sub>2</sub>), a greenhouse gas, into useful materials, as well as other "green" methods that are conducted in water.

### **Alexander M. Klibanov**

The Klibanov group has been working on improved nonviral nucleic acids delivery vectors for gene therapy; bifunctional multivalent inhibitors of influenza viruses; examination of the effect of radiofrequency radiation on enzymes, vaccines, and live cells; and polymeric materials coatings killing bacteria and viruses on contact.

### **Stephen J. Lippard**

The Lippard group focused on soluble single-walled carbon nanotubes that were functionalized with cisplatin to carry this potent anticancer drug more efficiently into cells and to target tumors via the folate receptor. A cationic platinum complex that forms DNA monofunctional adducts was identified as a promising new agent to treat colorectal cancer. The group's fluorescent nitric oxide sensor was instrumental in identifying NO as a novel antibiotic target for anthrax and *Staphylococcus aureus* (including methicillin-resistant *S. aureus*).

### **Mohammad Movassaghi**

The Movassaghi group has continued to focus on the development of new strategies and technologies for complex molecule synthesis. They have completed and reported the total synthesis of three dimeric and complex diketopiperazine alkaloids using their

cobalt-promoted dimerization strategy for complex alkaloid synthesis. Also, they have begun to examine their proposed oxidative rearrangement strategy for the preparation of a new subfamily of complex alkaloids containing challenging stereochemical features. The hallmark of their syntheses is the unparalleled efficiency and exquisitely high level of stereochemical control. In the context of their synthetic studies the group has developed new chemical transformations, including the first catalytic and asymmetric synthesis of monoalkyl diazenes from allylic electrophiles. 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 has used ultrashort pulses of light to achieve optical control over most types of collective modes of condensed matter, including acoustic waves of all frequencies and wavelengths, crystal lattice vibrations, and excitonic electronic excited states. Optical generation of compressional and shear acoustic waves in glass-forming liquids has revealed the dynamics of collective structural change in viscoelastic materials. Optical generation of large-amplitude polar lattice vibrations in ferroelectric crystals has revealed anharmonic lattice properties and yielded high-power terahertz electromagnetic pulses that have a wide range of fundamental and practical applications. Optical generation of coherent electronic responses in semiconductor nanostructures has permitted direct observation of correlated multielectron states called biexcitons. In each case, novel optical control over collective modes has permitted novel observations of collective dynamical behavior involving those modes.

### **Sarah E. O'Connor**

The O'Connor group's research has focused on elucidating and reengineering the biosynthetic pathway of terpene indole alkaloids, a complex metabolic pathway responsible for the production of hundreds of pharmaceutically important alkaloid natural products. They have shown that this pathway can support the production of "unnatural" natural products and have created a transgenic cell culture that has been engineered to produce "unnatural" products. Current efforts are focused on assessment of the biological activity of the unnatural products, further reengineering of the pathway in the plant Madagascar periwinkle, and identification of additional genes involved in the pathway.

### **Richard R. Schrock**

The research activities of the Schrock group lie in four areas: (1) multiple metal-carbon bonds, metallacycles, and catalysis; (2) enantioselective metathesis reactions and their applications in organic chemistry (in collaboration with A. Hoveyda at Boston College); (3) high oxidation state dinitrogen complexes and the catalytic reduction of dinitrogen; and (4) catalysts for living ring-opening metathesis polymerization and the cyclopolymerization of 1,6-heptadiynes to yield polyenes.

**Robert J. Silbey**

The Silbey group is trying to theoretically understand the mechanism of energy transfer in photosynthetic antenna complexes such as those found in certain bacteria. They have modeled the process using a quantum mechanical picture including the interaction of the excitations with vibrational modes and disorder. The group has been able to fit the experiments on energy transfer and spectroscopy with an effective Hamiltonian. In addition, they have found that the structure of the antenna complex makes it robust against energy changes in the environment of the chlorophyll molecules.

**Timothy M. Swager**

The Swager group has developed novel chemical sensors based on carbon nanotubes capable of parts per billion detection of explosives and chemical weapons. These sensors have greatly improved selectivity relative to other chemiresistive systems and are even capable of discriminating between hydrocarbon isomers. Other advances from the Swager group include the formation of superior materials for ballistic protection and novel chromophores for use in solar luminescent concentrators.

**Alice Y. Ting**

Alice Ting's lab is developing fluorescent reporters for live cell imaging. This past year, her group developed new technologies for chemical probe targeting to intracellular proteins, protein-protein interaction detection, and neuronal synapse detection. The last technology has been used to study the molecular mechanism of neurexin-neurologin interactions in the development and maturation of new synapses.

**Andrei Tokmakoff**

The Tokmakoff group studies time-dependent changes of molecular structure in chemical reactions and biophysical processes. Ultrafast two-dimensional infrared spectroscopy and modeling with molecular dynamics simulations were used to understand protein folding processes and proton transfer in aqueous hydroxide solutions. They are also using these and other time-resolved spectroscopies to study the mechanism of proton-coupled electron transfer along hydrogen bonds, and understand the interactions of proteins and peptides with water.

**Troy Van Voorhis**

Research in the Van Voorhis group has focused on several major topics in the past year: (1) modeling bond-breaking and proton-coupled electron transfer with density functional theory, (2) simulating transient charge transfer dynamics with semiclassical techniques, (3) understanding the fundamental principles of molecular conductance, and (4) developing techniques for the description of intermolecular interactions, in particular solvent-solute interactions.

**Timothy M. Swager**

**Department Head**

**John D. McArthur Professor**

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