Department of Chemistry

This report summarizes achievements and noteworthy events during the 2009–2010 academic year for Chemistry Department faculty, students, and staff at the Massachusetts Institute of Technology.

Department faculty currently consists of 31 full-time faculty: three assistant, four associate, and 24 full professors, one of whom is also an Institute Professor. Of the department's 12 emeritus professors, one is also an Institute Professor. In addition to research in biological, inorganic, organic, and physical chemistry, in the past year the Chemistry Department continued its strong programs in undergraduate and graduate education, with 211 graduate students, 133 postdoctoral researchers, and 92 undergraduate chemistry majors.

On July 1, 2010, Sylvia T. Ceyer, the John C. Sheehan professor of chemistry, will succeed Timothy Swager, John D. MacArthur professor of chemistry, as head of the department. John Essigmann, William R. and Betsy P. Leitch professor of chemistry and biological engineering, will replace Professor Ceyer as associate department head. At the same time, Mircea Dincă will join the faculty as assistant professor, and Mohammad Movassaghi and Troy Van Voorhis will assume the rank of associate professor with tenure.

Faculty Awards and Honors

Buchwald Received Esselen Award

Stephen L. Buchwald, the Camille Dreyfus professor of chemistry, was awarded the 2010 Gustavus J. Esselen Award for Chemistry in the Public Interest from the Northeastern Section of the American Chemical Society (ACS). The Esselen Award is presented annually to recognize a US or Canadian chemist whose scientific and technical work has contributed to the public wellbeing and has thereby communicated positive values of the chemical profession. Professor Buchwald's award recognizes his major impact on medicinal chemistry through his development of palladium- and copper-catalyzed processes to form carbon-nitrogen and carbon-oxygen bonds. These catalysts are used daily by the discovery groups of nearly every major pharmaceutical company worldwide. His catalysts have enabled the synthesis of novel, promising small-molecule drugs that target a wide range of diseases. His catalysts have also been instrumental in developing novel organic semiconductors and a wide range of other nonmedical chemical syntheses.

According to Thomas Reuters Essential Science Indicators, Professor Buchwald is the most cited chemist in the world, per paper, for the period January 1, 1999–August 31, 2009 (http://www.timeshighereducation.co.uk/story.asp? sectioncode=26&storycode=409 418&c=1).

Degen Won 2009 PNAS Cozzarelli Prize

Assistant professor Christian Degen and his coworkers at IBM were awarded the 2009 PNAS Cozzarelli Prize during the National Academy of Sciences (NAS) Annual Meeting on April 25, 2010, in National Harbor, MD, for their paper entitled "Nanoscale Magnetic Resonance Imaging." Papers selected for the Cozzarelli Prize are chosen from more than 3,700 research articles published by the *Proceedings of the National Academy of Sciences* (PNAS) in 2009 and represent the six broadly defined classes under which NAS is organized.

Drennan Received HHMI Professorship

Professor Catherine L. Drennan is one of 13 faculty members from around the nation to be named a Howard Hughes Medical Institute (HHMI) professor in the 2010 round of awards. Launched in 2002, the HHMI Professors Program recognizes accomplished research scientists who are also deeply committed to making science more engaging for undergraduates. Drennan also holds a prestigious HHMI investigator post for her excellence and innovation in research. She is the only individual in the country to be named both an HHMI professor and an HHMI investigator.

Griffin Awarded ISMAR Prize

The International Society of Magnetic Resonance (ISMAR) awarded its 2010 triennial prize to Robert G. Griffin, professor of Chemistry and director of MIT's Francis Bitter Magnet Laboratory, for his achievements in the field of magnetic resonance. Griffin has made outstanding contributions to nuclear magnetic resonance (NMR) spectroscopy, in particular his successful development of high-field dynamic nuclear polarization (DNP) as a practical method for sensitivity enhancement in sold-state NMR with magic-angle spinning. Other contributions include the design and construction of novel instrumentation for DNP and the use of nitroxide biradicals to improve DNP sensitivity. Griffin's group recently demonstrated the ability of DNP to detect and characterize intermediates in the bacteriorhodopsin photocycle, the widely studied prototype of a ubiquitous family of light-driven ion pumps and a model for other members of the versatile family of retinal pigments, including the G-protein-coupled receptors in the visual system.

Imperiali Elected to NAS

Professor Barbara Imperiali has been elected to NAS in recognition of her distinguished and continuing achievements in original research. Election to NAS is considered a top honor for those in science and engineering.

Lippard Honored with Pauling Medal, Centenary Medal, and Breslow Award

On November 7, 2009, professor Stephen Lippard was presented with the Linus Pauling Medal by professor Carl Wamser, at Linus Pauling's alma mater, Portland State University.

The Pauling Medal recognizes outstanding achievement in chemistry and is presented annually by the Puget Sound and Portland, OR, sections of ACS. The award is named after two-time Nobel laureate Linus Pauling, a native of the Pacific Northwest. Professor Lippard joined John Waugh as the second faculty member in the department to have received this prestigious award.



Professor Carl Wamser (Portland State University) congratulates professor Stephen J. Lippard at the Pauling Medal award ceremony, November 7, 2009

Professor Lippard's lecture at the award ceremony was titled "Understanding and Improving Platinum Anticancer Drugs." Professors Christopher Cummins and Daniel Nocera from the department also spoke on this occasion, along with professor Wes Sundquist of the University of Utah, a former Lippard graduate student.

In 2010 Professor Lippard was honored with the Centenary Medal by the Royal Society of Chemistry in the UK for his pioneering studies of biological interactions involving metal ions, with a particular focus on the reactions, and physical and structural properties of metal complexes.

ACS recognized Professor Lippard at their 239th Annual Meeting with the 2010 Ronald Breslow Award for Achievement in Biomimetic Chemistry.

In May 2010, at its commencement exercises, the University of South Carolina conferred an honorary doctorate of science upon Professor Lippard for his contributions as a scientist and educator in inorganic and bioinorganic chemistry. Federal Reserve chairman Ben Bernanke and Pulitzer Prize—winning columnist Eugene Robinson were among the other honorees.

Nocera Received Honorary Degree from Michigan State University

Henry Dreyfus professor of energy and professor of chemistry Daniel Nocera received an honorary doctorate of science at Michigan State University at its commencement exercises on May 7. Emil Boc, prime minister of Romania, and Joseph Kennedy II, were among the other honorees.

Steinfeld Named AAAS Fellow

Professor emeritus Jeffrey I. Steinfeld was one of eight professors from MIT named as a fellow of the American Association for the Advancement of Science (AAAS) in 2010. Fellows are recognized by their peers for their scientifically or socially distinguished efforts to advance science and its applications.

Stubbe Recognized with National Medal of Science, Franklin Medal in Chemistry, and Welch Award in Chemistry

On October 7, 2009, in a ceremony held at the White House, President Barack Obama presented professor JoAnne Stubbe, Novartis professor of chemistry and professor of biology, with the National Medal of Science. The award honors her work understanding the mechanisms of enzymes that play an essential role in DNA replication and repair. On learning the news, professor Stephen Lippard, a 2004 National Medal of Science recipient, called Professor Stubbe "one of the top few mechanistic biochemists of her generation. There are



President Barack Obama and professor JoAnne Stubbe at the National Medal of Science Ceremony at the White House, October 7, 2009

few people with her drive for understanding and insistence on accuracy in experimental work." MIT president Susan Hockfield also praised Stubbe, calling her "a scientist's scientist: fiercely intelligent, doggedly curious, and unbending in her pursuit of truth."

On October 19, 2009, the Franklin Institute announced that Professor Stubbe had been awarded the 2010 Benjamin Franklin Medal in Chemistry for "uncovering the intricate processes by which cells safely use free radicals, for developing new cancer treatments, and for improving the production of environmentally friendly biodegradable polymers."

Also in October, Professor Stubbe won the 2009 Prelog Medal, an award given annually by the Swiss Federal Institute of Technology (also known as ETH-Zürich) to one individual who has contributed significantly to the area of stereochemistry within the field of organic chemistry. ETH-Zürich honored Professor Stubbe with the Prelog Medal for her work on understanding how ribonucleotide reductases work. With this honor, she joins an elite group of chemists that includes several Nobel laureates.

At the annual ACS meeting, Professor Stubbe was recognized by the Biophysical Society with the 2010 Murray Goodman Memorial Prize.

Capping a year of impressive honors, on May 13, 2010, Professor Stubbe was cowinner of the Welch Award in Chemistry with Christopher T. Walsh, Hamilton Kuhn professor of biological chemistry and pharmacology at Harvard Medical School, for groundbreaking work explaining how enzymes have evolved to carry out difficult and

ingenious chemistry critical to life. Christopher Walsh is a former member of the MIT faculty, where he served as head of the Chemistry Department. Their research has laid the groundwork for therapeutic advances in medicine, particularly in the treatment of cancer. Stubbe is the second MIT faculty member to win the award after Alexander Rich, who won in 2008.

Ting Received ACS Eli Lilly and Cope Awards

Alice Y. Ting, associate professor of chemistry, was granted the Eli Lilly Award by ACS's Division of Biological Chemistry for her achievements in biological chemistry of unusual merit and independence of thought and originality.

In recognition of her use of lipoic acid ligase to attach biophysical probes to proteins with excellent site specificity for use in live cell imaging, ACS also awarded Professor Ting with the 2010 Arthur C. Cope Scholar Award.

Other Departmental News

Dincă Joined Faculty

Assistant professor Mircea Dincă came to the Department of Chemistry in 2008 as a postdoctoral associate in the Nocera group, following his doctoral studies at the University of California at Berkeley. The Dincă group focuses on research related to the storage and transport of energy, as well as on global environmental concerns. Central to the lab's work is the manipulation of electrochemical and photophysical processes in inorganic materials, with an emphasis on microporous materials.

ACS President-elect's Seminar

Chemistry Department alumnus Joseph S. Francisco PhD '83, president-elect of the American Chemical Society and William E. Moore distinguished professor of chemistry at Purdue University, was invited to give a special physical chemistry seminar on September 29, 2009. Professor Francisco met with physical chemistry faculty, including his doctoral advisor, professor emeritus Jeffrey Steinfeld, and visiting Martin Luther King professor John Harkless, as well as associate provost Wesley Harris and School



Professor Timothy M. Swager (Chemistry Department head), Joseph S. Francisco (Chemistry PhD '83), and professor emeritus Jeffrey I. Steinfeld outside the 6-120 lecture hall on September 29, 2009

of Science dean Marc Kastner. An informal luncheon was held with the MIT chapter of the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChe). His talk, entitled "Structure and Reactivity of Radical-Molecule Complexes: New Frontier of Atmospheric Chemistry," was attended by students and faculty from the departments of Chemistry, Physics, and Chemical Engineering.

Martin Luther King Visiting Professor

Professor John Harkless, Martin Luther King visiting professor, joined the MIT Chemistry Department for the academic year 2009–2010. Professor Harkless received his BS in chemistry and mathematics from Morehouse College in 1995. He graduated from the University of California at Berkeley with a PhD in theoretical chemistry in 2001, after which he spent a year as a National Research Council postdoctoral researcher in the Computational Chemistry Group at National Institute of Standards and Technology.

His research at Howard focuses on quantum Monte Carlo wave function development, electronic structure of metallic systems, and electronic excitations. His scientific articles have appeared in the *Journal of Chemical Physics*, the *Journal of Physical Chemistry A*, and the *International Journal of Quantum Chemistry*. At Howard, he teaches general chemistry, computational methods in chemistry, and physical chemistry. He is vice president of NOBCChe and has been responsible for the NOBCChe Science Bowl and Science Fair for high school students.

Peter Curtin

With great sadness, the department reports that on Saturday, October 10, 2009, Peter Curtin, a second-year graduate student in the Nocera group, passed away while running the Baltimore Marathon. He was engaged in collaborative research with the Bawendi lab on sensors designed to assess the health of a tumor and had been recently granted a National Defense Science and Engineering Graduate Fellowship.

Before entering MIT, Curtin earned his AB in chemistry with highest honors from Princeton University in 2008. His family has established the Peter N. Curtin, Class of 2008, Memorial Fund in his memory to support undergraduates in the Princeton Department of Chemistry. Donations in Peter's memory may be made out to Princeton University with the note, Peter N. Curtin, Class of 2008, Memorial Fund, and mailed to Helen Hardy, Princeton University, Alumni and Donor Relations, PO Box 5357, Princeton, NJ 08543.

Infinite Kilometer Awards

Tyler Brezler, administrative assistant to professors Rick Danheiser and Mohammad Movassaghi, and Gang Liu, PhD, project technician, were recognized with School of Science Infinite Kilometer Awards. The Infinite K Award recognizes the dedication of staff at all levels who "go the extra kilometer" to help members of the MIT community and make activities at the Institute successful.

MIT Excellence Award

This March, all three members of the Chemistry Education Office, senior administrative assistant Susan Brighton, academic administrator Melinda Cerny, and administrative assistant Mary Turner, were recognized with the MIT Excellence Award in the category of "Serving the Client." The team was described as a "group of miracle workers" who assist students in the department in every aspect of their academic careers, guaranteeing that no student or faculty member has to go elsewhere for an answer about degree requirements, classes, or Chemistry Department extracurricular activities.

Infinite Mile Award

Dr. John Dolhun, instructor in the Undergraduate Laboratories, received a 2010 Infinite Mile Award. The awards, bestowed by the School of Science, are for those individuals whose outstanding accomplishments and willingness to far beyond the extra mile for coworkers, the School, and the MIT community make them well deserving of recognition.

Twardowski Appointed Undergraduate Laboratory Director

Dr. Mariusz Twardowski, who became acting director of the Undergraduate Laboratory when the previous director retired in 2008, was officially appointed director of the Undergraduate Laboratory.

Dr. Twardowski, who received his PhD from the University of Illinois at Urbana-Champaign, joined the Chemistry Department as the director of Undergraduate Research-Inspired Experimental Chemistry Alternatives (URIECA) in 2007. Plans for the undergraduate lab include working with URIECA faculty to improve the curricula as new developments in chemistry present teaching opportunities and continuing to expand the lab's instrumentation and equipment. Dr. Twardowski has received many inquiries from other universities and research institutions about our department's curriculum and hopes it can serve as a useful model for others as they revamp their lab programs.

Speakers in Named Lecture Series

During the 2009–2010 academic year, the department welcomed the following speakers in named lectures:

September 11, 2009 – Andreas Pfaltz (University of Basel) – Wyeth Lecture in Organic Chemistry

September 14, 15, and 17, 2009—Wilson Ho (University of California at Irvine)—Arthur D. Little Lecture Series in Physical Chemistry

October 29, 2009—Laura Kiessling (University of Wisconsin at Madison)—Büchi Lecture in Organic Chemistry

November 17 and 18, 2009—David Milstein (Weizmann Institute of Science)—Arthur D. Little Lecture Series in Inorganic Chemistry

January 14 and 15, 2010—Takuzo Aida (University of Tokyo)—Merck-Pfister Lectures in Organic Chemistry

March 25, 2010—André Charette (University of Montreal) and Gregory Vite (Bristol-Myers Squibb)—Bristol-Myers Squibb Lectures

April 1, 2010—Jeffrey Aubé (University of Kansas) and David J. Calderwood (Abbott Bioresearch Center)—Abbott Lectures in Organic Chemistry

April 8, 2010—Mikiko Sodeoka (RIKEN)—Boehringer-Ingelheim Lecture in Organic Chemistry

April 13, 2010—Stephen J. Benkovic (Pennsylvania State University)—T.-Y. Shen Lectures

April 22, 2010—Bradley S. Moore (Scripps Institute of Oceanography) and John Tallarico (Novartis Institutes of Biomedical Research)—Novartis Lectures in Organic Chemistry

May 18 and 19, 2010—Kenneth N. Raymond (University of California at Berkeley)—Davison Lectures in Inorganic Chemistry



Professor JoAnne Stubbe, professor T.-Y. Shen, and professor Stephen Benkovic at the T.-Y. Shen Lecture, April 13, 2010

Chemistry Education

Undergraduate Education

Serving the Institute

The Department of Chemistry provides key educational service to the Institute. During academic year 2009–2010, the Department of Chemistry trained 1,861 MIT students in the areas of biochemistry, inorganic, organic, and physical chemistry. The department also was home for 64 students in the Undergraduate Research Opportunities Program (UROP), which provided important mentoring relationships for students from a number of departments, including chemistry, biology, mathematics, physics, chemical engineering, electrical engineering, materials science, and mechanical engineering.

Chemistry Majors

As of July 2010, the department will have a total of 92 majors. The past two years we have seen class sizes growing from the mid-20s to the low- to mid-30s. In February and June 2010, a total of 28 students received SB degrees in chemistry. In exit surveys this year, we found that the Class of 2010 is showing a new trend in post-SB plans. A majority of our seniors (65 percent) are still bound for graduate school, but this year 18 percent have chosen employment and only17 percent plan to attend medical school. This decline in premed majors is a significant decline from years past, when students were almost equally divided between graduate school and medical school.

Cambridge-MIT Exchange Program

This year we had two chemistry majors spend the year in England and we hosted three Cambridge students in the department. With the implementation of the new URIECA schedule, more chemistry majors are finding it easier to schedule their lab classes so that they can spend their junior abroad.

Student Awards and Recognition

The 2010 Undergraduate Senior Recognition and Awards Banquet was held on May 13 at the R&D Common Era in the Stata Center. The following awards were presented:

Alpha Chi Sigma Award for outstanding achievement in scholarship, research, and service to the department—Michael R. Blaisse, Sidney E. Creutz

Merck Index Award for outstanding scholarship—Chung-Yang (Dennis) Huang, Deborah C. Markham, Ke Zhang

Research Award for outstanding contributions in the area of research—Kevin Hwang, Xin Jin, Fan Liu

Strem Award in recognition of the best undergraduate research presentation at the UROP Symposium on April 24, 2010—Fan Liu, Katharine E. Silberstein

Frederick D. Greene Teaching Award for outstanding contributions in the area of teaching—Elizabeth M. Iffrig, Sarah B. King

ACS Analytical Chemistry Award for an outstanding analytical chemist (junior year)—Andrew J. Musacchio

Department of Chemistry Service Award for significant contributions in the area of service to the department—Angela Y. Zhu

Sophomore Achievement Award for outstanding performance in academics, research, and service to the department—Anna Levina, Daniel S. Levine, Anupong Tangpeerachaikul

Hypercube Scholar Award in recognition of outstanding contribution to the advancement of computational chemistry—Christopher A. Kennedy

CRC Press Freshman Chemistry Achievement Award for outstanding academic achievement in chemistry—Linh T. Bui

This year the Barry M. Goldwater Award for Excellence in Education was awarded to junior Alex Vai.

Chemistry majors who served this year as teaching assistants and tutors as well as "Course V Ambassadors" and "Chemistry Magic Show" performers were also recognized at the senior banquet. (Ambassadors are majors who meet with high school students, give them a tour of their UROP lab, and discuss life as a chemistry major at MIT. The Chemistry Magic Show is a road show for elementary school-aged children.)

Teaching—Bina Choi: Fall, 5.07; Sid Creutz: Fall, 5.112, Spring, 5.62; Jonathon Gunn: Fall, 5.111; Elizabeth Iffrig: Fall, 5.12, Spring, 5.12; Sarah King: Fall, 5.12, Spring, 5.12; Rich Whalley: Fall, 5.12; Ke Zhang: Fall, 5.60, Spring, 5.12; Angela Zhu: Fall, 5.07

Tutoring—Mike Blaisse: Fall, 5.60; Marie Herring: Spring, 5.111; Morgan Houston: Fall, 5.111/2; Brian Lee: Fall, 5.13; Daniel Levine: Fall, 5.12, Spring, 5.111; Katie Mingo: Spring, 5.111; Juliann Reardon: Fall, 5.13, Spring, 5.03; Dale Robinson: Fall, 5.111/2; Ryan Rosario: Spring, 5.111; Katie Silberstein: Fall, 5.111/2, Spring, 5.03; Mia Shandell: Spring, 5.12; Mee Tangpeerachaikul: Fall, 5.12, Spring, 5.12; Victoria Wang: Fall, 5.12, Spring, 5.12; Yuxin Xie: Fall, 5.12; Angela Zhu: Spring, 5.111

Course V Ambassadors—Mike Blaisse, Jon Gunn, Zach Hynes, Sarah King, Daniel Levine, Galina Mamaliga, Brian McCarthy, Kasey Rowe, Mia Shandell, Katie Silberstein, Samuel Thompson

Chemistry Magic Show—Marie Herring, Daniel Levine, Brian McCarthy, Victoria Wang



Front Row: Angela Zhu Second Row: (LtoR) Sid Creutz, Xin Jin, Alexandra Barry, Kasey Rowe, Katie Silberstein, Sarah King, Victoria Lee, Fan Liu

Seniors Recognition Banquet, May 13, 2010





Back Row: (LtoR) Kevin Hwang, C. Ryan Tait, Bill Phipps, Dale Robinson, Katie Mingo, Liz Iffrig, Mike Blaisse, Ke Zhang, ChungYang (Dennis) Huang

Seniors Recognition Banquet, May 13, 2010. Front row: Angela Zhu; second row (L to R): Sid Creutz, Xin Jin, Alexandra Barry, Kasey Rowe, Katie Silberstein, Sarah King, Victoria Lee, Fan Liu; back row (L to R): Kevin Hwang, C. Ryan Tait, Bill Phipps, Dale Robinson, Katie Mingo, Liz Iffrig, Mike Blaisse, Ke Zhang, Chung Yang (Dennis) Huang

Undergraduate Research Opportunities Program

UROP remains the capstone experience for our undergraduates. With over 90 percent of our majors working in a research group (the majority in chemistry) at least once during their degree program, they have the unique opportunity to conduct research alongside faculty, postdocs, and graduate students.

UROP Publications 2009-2010

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

"A fluorophore ligase for site-specific protein labeling inside living cells." *PNAS* 2010, 107, 10914-10919. C. Uttamapinant, K. A. White, H. Baruah, **S. Thompson**, M. Fernández-Suárez, S. Puthenveetil, and A. Y. Ting.

"Conjugated Polymers that Respond to Oxidation with Increased Emission." Dane, E. L.; **King, S. B.**; Swager, T. M. *Journal of the American Chemical Society*, 2010, 132, 7758-7768.

Effective Hamiltonians, in Handbook of High Resolution Spectroscopies. R. W. Field, J. H. Baraban, S. H. Lipoff, and **A. R. Beck**, M. Quack and F. Merkt (editors), John Wiley and Sons (2010).

"Manganese displacement from Zinpyr-1 allows zinc detection by fluorescence microscopy and magnetic resonance imaging." Youngmin You, Elisa Tomat, **Kevin Hwang**, Tatjana Atanasijevic, Wonwoo Nam, Alan P. Jasanoff, and Stephen J. Lippard, *Chemical Communications*, 4139-4141 (2010).

"Modeling the Syn Disposition of Nitrogen Donors in Non-Heme Diiron Enzymes. Synthesis, Characterization, and Hydrogen Peroxide Reactivity of Diiron(III) Complexes with the Syn N-Donor Ligand H₂BPG₂DEV." Simone Friedle, Jeremy J. Kodanko, **Anna J. Morys**, Takahiro Hayashi, Pierre Moënne-Loccoz, and Stephen J. Lippard. *Journal of the American Chemical Society*, 131, 14508-14520 (2009).

"Photoaffinity Isolation and Identification of Proteins in Cancer Cell Extracts that Bind to Platinum-Modified DNA." Evan R. Guggenheim, Dong Xu, Christiana X. Zhang, **Pamela V. Chang**, and Stephen J. Lippard. *ChemBioChem*, 10, 141-157 (2009).

"Preparation of Mammalian Expression Vectors Incorporating Site-Specifically Platinated-DNA Lesions." Wee Han Ang, **William Wesley Brown**, and Stephen J. Lippard, *Bioconjugate Chemistry*, 20, 1058-1063 (2009).

"Stille Cross-Coupling Reactions of Aryl Mesylates and Tosylates Using a Biarylphosphine Based Catalyst System." Naber, J.R.; Fors, B.P.; Wu, X.; Gunn, J. and Buchwald, S.L. *Heterocycles* 2010, 80, 1215-1226. (PMC Journal-In Process)

"Transcription Inhibition by Platinum DNA Cross-links in Live Mammalian Cells." Wee Han Ang, **MyatNoeZin Myint**, Stephen J. Lippard. *Journal of the American Chemical Society*, 132, 7429-7435 (2010).

Course V Events

The majors are active promoters of chemistry and were on hand to talk with freshmen at the Academic Expo in August, 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), performed for middle school-aged girls at a Society of Women Engineers event, and took their show on the road to the Eliot Elementary School in the spring.

Graduate Education

Graduate Student Teaching Assistants

We continue to offer an extensive training program for teaching assistants at the beginning of the fall semester. Led by Dr. Sanjoy Mahajan of the MIT Teaching and Learning Lab, Professor Catherine Drennan, Dr. Beth Vogel, and experienced graduate

students, new teaching assistants (TAs) prepare for their teaching responsibilities in the classroom and lab through a series of workshops and microteaching. The workshops cover specifics on lesson planning and engaging students in active learning, as well as discussion about classroom diversity and one-on-one TA/student interactions.

We had an outstanding team of teaching assistants this year. Engaged, enthusiastic, and willing to try new things, these TAs were outstanding in fulfilling their teaching requirement. The student evaluation results were excellent. On a scale of 1 to 7, 91 percent of our TAs received a 5.0 or better, and 59 percent received a 6.0 or higher. TAs do not receive these kinds of accolades from our students just for showing up. Indeed, MIT undergraduates have high expectations for their TAs, so to receive scores like these says quite a lot about our graduate students' commitment to chemistry and to encouraging the next generation.

Two student comments typify the sentiments shared in the evaluations. The first is about a lab TA; the second is about a recitation TA.

"Everything was so much clearer after she presented. She also said hi to me in the hallways outside of class, which I thought was nice—it let me know that she cared about me as a person and student in general rather than just cared when she was officially obligated to help. That sort of positive, professional relationship also fosters hard work; in a way I almost felt like I wanted to do well because I didn't want to disappoint her after she had put in so much effort to help me."

"...an amazing TA. She answered our questions carefully and succinctly in class, and quickly responded with book references, examples, and explanations when I asked questions via email. She encouraged us to participate in recitation by asking us questions and having us come up to the board to work through problems. Her use of colored chalk also helped emphasize important points. She clearly wants all of her students to succeed, and was willing to change her office hours and arrange meeting times for students who needed help. When things in the book seemed to contradict explanations given in lecture, Lisa would quickly point out differences between the two, explaining how both were correct."

Graduate Awards and Fellowships

Omar Ahmad (Movassaghi Group)—Bristol-Myers Squibb Fellowship in Synthetic Organic Chemistry

Kurt Armbrust (Jamison Group)—National Science Foundation (NSF) Graduate Research Fellowship

Kevin Chang (Degen Group)—C.P. Chy and Y. Lai Summer Graduate Fellowship

Jian Cui (Bawendi Group) – NSF Graduate Research Fellowship

Peter Curtin (Nocera Group)—National Defense Science and Engineering Graduate Fellowship Fellowship

Brett Fors (Buchwald Group) — Amgen Summer Graduate Fellowship

Alexander Fox (Cummins Group)—Morse Travel Grant

Kelvin Frazier (Swager Group)—Daniel S. Kemp Summer Graduate Fellowship

Weslee Glenn (O'Connor Group)—NSF Fellowship

Sunkyu Han (Movassaghi Group) – EMD Serono Summer Graduate Fellowships

Wendy Iskenderian-Epps (Imperiali Group)—David A. Johnson Summer Graduate Fellowship

Xin Jin (Course 5, Year 4)—Novartis Summer Undergraduate Fellowship

Christopher Leon (Ceyer Group)—Natural Sciences and Engineering Research Council of Canada (NSERC) Scholarship; Martin Family Society of Fellows for Sustainability (MFSFS) Fellowship

Harris Liu (Nolan Group) - Strem Summer Graduate Fellowship

Zhe Lu (Fu Group)—2010 Goodwin Medal for "conspicuously effective teaching" by a graduate student

Pamela Lundin (Fu Group) — AY2010 Eli Lilly Graduate Fellowship in Organic Chemistry

Lisa Marshall (Bawendi Group)—David A. Johnson Summer Graduate Fellowship

Christopher Morten (Jamison Group)—EMD Serono Summer Graduate Fellowships

Tarun Narayan (Dinca Group)—C.P. Chy and Y. Lai Summer Graduate Fellowship

Benjamin Ofori-Okai (Degen Group)—Henry A. Hill Underrepresented Minority Graduate Fellowship

Barratt Park (Field Group)—2010 K. Narahari Rao Prize for Best Talk by Graduate Student at International Symposium on Molecular Spectroscopy

Semi Park (Lippard Group)—IMPI Award

Mike Pluth (Lippard Group)—National Institutes of Health Pathway to Independence Fellowship

Julia Robinson (Danheiser Group)—AY2010 AstraZeneca Graduate Fellowship in Organic Chemistry; David A. Johnson Summer Graduate Fellowship

Daniel Rowlands (Ceyer Group)—Corning Foundation Fellowship

Todd Senecal (Buchwald Group) — EMD Serono Summer Graduate Fellowship

Sarah Slavoff (Ting Group)—ACS Division of Organic Chemistry Fellowship; David A. Johnson Summer Fellowship

Georgiy Teverovskiy (Buchwald Group)—National Defense Science and Engineering Graduate Fellowship

Ryan Todd (Lippard Group)—Strem Summer Fellowship

Jessica Tanuwidjaja (Jamison Group) — AY2010 Novartis Graduate Fellowship in Organic Chemistry

Ye Tao (Degen Group)—George H. Büchi Summer Graduate Fellowship

Brett VanVeller (Swager Group)—David A. Johnson Summer Graduate Fellowship

Darcy Wanger (Bawendi Group)—Ann and Paul Steinfeld Memorial Summer Graduate Fellowship

Tom Willumstad (Danheiser Group)—Merck Summer Graduate Fellowship

Tengfei Zheng (Nolan Group)—Kenneth M. Gordon Fellowship; Norris Fellowship

Daniel Ziegler (Fu Group) — EMD Serono Summer Graduate Fellowship

Sue Zultanski (Fu Group) – Merck Summer Graduate Fellowship

Graduate Degrees Conferred

Doctoral and Master's Degree Recipients

Peter Allen, PhD (Bawendi)

Maksym Artomov, PhD (Chakraborty)

Mariya Barch, PhD (Matsudaira)

Marvin Bayro, PhD (Griffin)

Peter Bernhardt, PhD (O'Connor)

Julian Chan, PhD (Swager)

Jia Min Chin, PhD (Schrock)

Yoon-Aa Choi, PhD (Ting)

Timothy Cook, PhD (Nocera)

Brandi Cossairt, PhD (Cummins)

Cynthia Crosswhite, SM (Danheiser)

Nicole Davis, SM (Danheiser)

Seth Difley, PhD (Van Voorhis)

Alexander Fox, PhD (Cummins)

Simone Friedle, PhD (Lippard)

Ziad Ganim, PhD (Tokmakoff)

Kristin Glab, SM (Swager)

Annie King, PhD (Schrock)

Christoph Klieber, PhD (Nelson)

Andrew Lauer, PhD (Jamison)

Wenhao Liu, PhD (Bawendi)

Katherine Lovejoy, PhD (Lippard)

Galen Loving, PhD (Imperiali)

Elvedin Lukovic, PhD (Imperiali)

Rebecca Mayrhofer, SM (Griffin)

Lindsey McQuade, PhD (Lippard)

John Naber, PhD (Buchwald)

Gautham Nair, PhD (Bawendi)

Christine Phillips, PhD (Drennan)

Sean Roberts, PhD (Tokmakoff)

Erika Robertson, SM (Field)

Gagan Saini, PhD (Nelson)

Wenchao Sheng, PhD (Shao-Horn)

Dustin Siegel, PhD (Movassaghi)

Meiliana Tjandra, PhD (Movassaghi)

Ryan Todd, PhD (Lippard)

Daniel Turner, PhD (Nelson)

Ivan Vilotijevic, PhD (Jamison)

Keith Wampler, PhD (Schrock)

Jun Wang, PhD (Stubbe)

Felix Westerhaus, SM (Buchwald)

Brian Wong, PhD (Lippard)

Research Highlights

Moungi Bawendi

Professor Bawendi and his students developed a novel spectroscopic method to measure the average linewidth of single chromophores (dyes or quantum dots) in solution by combining fluorescence correlation spectroscopy and photon correlation Fourier spectroscopy. This method can also extract out the dynamical behavior of an average single molecule fluorescence spectrum in solution down to an unprecedented time scale of ~30 nanoseconds. This method has potential for the study of dynamics of biological molecules in live cells with unprecedented time resolution. Professor Bawendi collaborated with professor Vladimir Bulovic in demonstrating novel quantum dot-based electro-optic devices, including light emissive, photodetecting, and photoconductive devices. Professor Bawendi and his students developed novel small and stable coatings for the biological application of quantum dots. They used these novel structures in collaborations with the Nocera group at MIT and the Jain group at Massachusetts General Hospital to demonstrate the use of quantum dots for the study of tumor microenvironments.

Arup Chakraborty

Robert T. Haslam professor Arup K. Chakraborty had a productive year in teaching and research. In research, he continued to make advances in T-cell signaling and T-cell repertoire development, and launched new efforts on T-cell lymphomas and

the human immune response to the human immunodeficiency virus (HIV). In these endeavors, his lab brought together statistical mechanical approaches rooted in physics and engineering with experimental studies carried out by collaborators who are basic immunologists and clinicians. Perhaps the most significant study emerging from Chakraborty's laboratory this year is the discovery of a new effect that contributes to the ability of people with certain genes to control HIV infections. This new effect originates from differences during T-cell development that result in people with certain genes having a more cross-reactive T-cell repertoire, which can mount strong immune pressure on the infecting HIV strain and mutants that emerge during infection. The paper describing this work was published in *Nature* and was the subject of more than 100 news stories in scientific journals and the international popular press (such as TIME, the BBC, Voice of America, and so on). Chakraborty continues to be a member of the steering committee of the Ragon Institute of Massachusetts General Hospital, MIT, and Harvard. He is also the leader of one of the four projects that are a part of the recently established National Institutes of Health-funded Physical Science-Oncology Center at MIT. Chakraborty continues to teach subjects in chemical engineering and chemistry and serves the Institute and the profession in numerous ways.

Christopher C. Cummins

Highlights from the Cummins lab during the past year have stemmed from the report of a niobium-based method for synthesis of the tetra-atomic AsP₃ molecule (*Science* 2009, 323, 602). Though composed of only two elements and four atoms, this method is the first preparative procedure for the synthesis of this molecule, which is isolable via sublimation as a pure substance. In two full papers the Cummins group has now described in detail the reactivity patterns (*Journal of the American Chemical Society* 2009, 131, 15501-15511), as well as the structural, spectroscopic and physical properties of AsP₃ (*J. Am. Chem. Soc.* 2010, 132, 8459-8465). Its synthesis and studies of AsP₃ have been recently highlighted in the German chemical newsmagazine, *Nachrichten Aus Der Chemie*.

Another important advance from the past year has been the development and publication of a ligand-based method for CO_2 fixation and reduction to CO (*J. Am. Chem. Soc.* 2010, 132, 2169-2171).

John M. Essigmann

John Essigmann's group designed a bifunctional toxicant in which a DNA-damaging agent was tethered to a ligand for the estrogen receptor. The molecule bound to DNA in vivo and then functionally displaced the endogenous estrogen receptor from its normal sites of action. The compound was seven times more persistent in ovarian cancer cells that expressed a normal level of the receptor than the same cells in which RNA interference was used to suppress the expression of the receptor. In other work, an antiviral agent designed initially in this laboratory has successfully reached phase IIa clinical trials; this molecule ablates viral populations by forcing the virus to exceed its error catastrophe limit.

Robert W. Field

Chirped pulse millimeter-wave spectroscopy is proving to be a revolutionary technique, combining the capability of searching a broad spectral region at high resolution. It is being used to observe "pure electronic" Rydberg-Rydberg transitions, which sample the anisotropic interactions between an electron and the molecular ion core to characterize the structure of a transition state by measuring the relative species/conformer/vibrational level populations of pyrolysis and photolysis products, to map the minimum energy acetylene-vinylidene isomerization path on the ground state potential surface.

Barbara Imperiali

Ongoing research focuses on protein glycosylation in selected prokaryotic pathogens, such as *Campylobacter jejuni*, *Neisseria meningitides*, and *Pseudomonas aeruginosa*, with the goal of understanding the roles of cell surface carbohydrates in human infectious diseases. In particular, emphasis is being placed on investigating the specific functions of unusual and highly modified carbohydrates in the glycoprotein conjugates of many pathogenic bacteria. Research also focuses on the application of innovative chemical tools for the study of biological systems. In particular, methods for sensitive and selective methods for diagnosing the dynamic fluctuations of enzyme activities, such as those of kinases, and protein/protein interactions are being developed for studies of cell migration, cell cycle control, and the regulation of synaptic plasticity.

Timothy F. Jamison

The Jamison group's research focuses on the discovery and implementation of new reactions for organic synthesis. Many of the transformations targeted are based on common structural motifs or functional group patterns present in molecules found in nature and/or pharmaceuticals. The group is also inventing reactions that convert carbon dioxide (CO_2) , a greenhouse gas, into useful materials; "green" methods that are conducted in water; and continuous-flow chemistry for pharmaceutical manufacturing.

Stephen J. Lippard

Using a cell-permeable porphyrin-based magnetic resonance imaging contrast agent, mobile zinc was imaged in the brains of live rodents. The membrane permeability, optical activity, and high relaxivity of the porphyrin-based contrast agent offers exceptional functionality for in vivo imaging.

Identification of protein-bound dinitrosyl iron complexes were identified by nuclear resonance vibrational spectroscopy, a powerful new methodology for studying protein active sites containing iron.

Mitaplatin, a potent fusion of cisplatin and the orphan drug dichloroacetate, was introduced as a new cancer drug candidate that selectively kills cancer cells instead of normal fibroblasts because of dual action at both the nucleus and the mirochrondrion of the cell.

Mohammad Movassaghi

The Movassaghi group's research program continues to focus on the development of new strategies and technologies for complex molecule synthesis. They have completed and reported the first total synthesis of 11,11'-dideoxyverticillin A, a complex epidithiodiketopiperazine alkaloid, representing the first such total synthesis of these compounds in 40 years since their initial isolation from nature. Recently, they have completed the enantioselective total syntheses of all six naturally occurring agelastatin alkaloids. The group's synthesis of agelastatin A is the shortest, most efficient, and the first bioinspired approach to this exciting alkaloid. The hallmark of the syntheses is their unparalleled efficiency and level stereochemical control in most complex settings, taking full advantage of the inherent chemistry of plausible biosynthetic intermediates. Additionally, the group has 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

The Nelson group developed novel methods for generating shaped femtosecond laser fields that include multiple beams in specified locations and multiple ultrashort pulses with specified optical phases and delay times. They used the methods to conduct the first multiple-quantum two-dimensional Fourier transform optical spectroscopy (2D FTOPT) measurements, analogous to multiple-quantum 2D FTNMR. The measurements revealed correlated multi-exciton states in GaAs quantum wells, allowing the first direct observations of biexcitons and triexcitons (correlated pairs and triplets of excitons) and showing that there were no significant higher-order correlations. The results elucidated the properties and the extent of multi-exciton correlations in this prototype system. Multi-exciton states play key roles in optical gain and other quantum well properties. The results were published in *Science* 2009, *Nature* 2010, *Journal of Chemical Physics* "Editors' Choice 2009," and *Accounts of Chemical Research* 2009.

Daniel G. Nocera

The Nocera group worked on an artificial photosynthesis system that uses sunlight to generate hydrogen gas that, in turn, can be used to power a hydrogen cell. The design, which approximates the energy-generating chemical reactions that happen naturally in plants, helps overcome what is cited as the most nagging problem of solar energy: the inability to generate electricity when the sun is not shining.

Elizabeth Nolan

In the past year, the Nolan group has initiated studies of interactions between antimicrobial peptides and metal ions.

Robert J. Silbey

Scientific activities with students and colleagues: published a number of research papers on energy transfer processes, especially those associated with chlorophyll complexes in photosynthetic organisms.

JoAnne Stubbe

The Stubbe group has developed Gemzar, a drug currently used in the treatment of advanced pancreatic cancer and non-small-cell lung carcinoma. The phosphorylated metabolites of this nucleoside interfere with many steps in nucleotide metabolism, including ribonucleotide reductases. This past year the group demonstrated that the diphosphate of Gemzar is a substoichiometric mechanism–based inhibitor of both human ribonucleotide reductases. While this compound acts like the classical mechanism–based inhibitors elucidated by the efforts of this lab, the added twist is that during inactivation the subunits of the enzyme become tightly associated. This novel mechanism likely plays a key role in its therapeutic efficacy.

A member of the Stubbe group, Joseph Cotruvo, discovered the first dimanganese ribonucleotide reductase, a unique target for pathogenic organisms.

Timothy M. Swager

The Swager research group has developed new, revolutionary methods for the detection of ionizing radiation using carbon nanotubes that have applications for national security. In particular, the methods allow for large-area real-time dosimeters to be constructed. Other innovations involve collaborations with professor Robert Griffin, director of the Francis Bitter National Magnet Laboratory, on the development of new agents for dynamic nuclear polarization. Dynamic nuclear polarization methods enable new magnetic resonance medical imaging that will allow for higher fidelity imaging of disease. Other ongoing projects in the Swager group are charting new frontiers in chemical and biological sensing, photovoltaics, structural materials, nanoelectronics, and electrochemical energy conversion methods.

Alice Y. Ting

Alice Ting's lab engineers reporters for live cell imaging. They have developed highly specific, minimally invasive reporters for imaging of protein trafficking and protein-protein interactions, at both the ensemble and single-molecule levels in living cells. Over the past year, her lab has applied these novel reporters to uncover new biological functions of the synaptic adhesion proteins neurexin and neuroligin.

Andrei Tokmakoff

The Tokmakoff group studies time-dependent changes of molecular structure during chemical reactions and biophysical processes. They do so by developing advanced time-resolved spectroscopy, which they combine with molecular dynamics simulations. They are using two-dimensional infrared spectroscopy to study the mechanism by which a proton is transported along hydrogen-bonding networks in water. They also have studied an array of biophysical dynamics problems, including the mechanism of insulin dimmer association, the structure of elastin-like peptides, conformational variation of peptides, and the folding of proteins and peptides.

Troy Van Voorhis

Research in the Van Voorhis group has focused on several major topics in the past year: 1) modeling reaction barriers and excited states using density functional theory, 2) constructing quantum mechanical/molecular mechanical models of organic semiconductor electronic structure, 3) describing conductance in metal-molecular metal junctions, and 4) developing techniques for the description of intermolecular interactions.

Timothy M. Swager Department Head

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