

Department of Chemistry

In the 2004–2005 academic year, the Chemistry Department continued its strong programs in undergraduate and graduate education. Associated with the department currently are 248 graduate students, 100 postdoctoral researchers, and 93 undergraduate chemistry majors. As of July 1, 2005, the Chemistry Department faculty will comprise 30 full-time faculty members including 5 assistant professors, 4 associate professors, and 21 full professors—one an Institute Professor. In the spring professors Jianshu Cao, Catherine L. Drennan, and Andrei Tokmakoff were promoted to associate professors with tenure, which will take effect on July 1, 2005. On February 1, 2005, the dean of Science, Robert J. Silbey, announced that Professor Timothy M. Swager will take over as the new department head on July 1, 2005. Professor Sylvia T. Ceyer will be the new associate department head, with executive authority over the department's educational programs. Professor Stephen J. Lippard and Professor Rick L. Danheiser stepped down as department head and associate department head, respectively, on June 30, 2005, after serving 10 years.

Major Faculty Awards and Honors

- Professor Stephen L. Buchwald received the 2005 Bristol-Myers Squibb Distinguished Achievement Award in Organic Synthesis
- Professor Sylvia T. Ceyer appointed as associate department head
- Professor Catherine L. Drennan received the Everett Moore Baker Memorial Award
- Professor Robert W. Field received the School of Science Dean's Educational and Student Advising Award
- Professor Stuart Licht was named Beckman Young Investigator
- Professor Stephen J. Lippard was elected for membership in the Leopoldina
- Professor Keith Nelson received the Class of 1960 Award for Innovation in Education
- Professor Daniel G. Nocera was elected a member of the American Academy of Arts and Sciences and was awarded the ITALGAS Prize for *Science and the Environment*
- Professor JoAnne Stubbe received the John Scott Award
- Professor Timothy M. Swager was appointed department head, received the ACS Carl S. Marvel Creative Polymer Chemistry Award, and was selected to be the John D. MacArthur Professor
- Professor Alice Y. Ting was named Alfred P. Sloan research fellow and was selected to receive a 2005 McKnight Technological Innovations in Neuroscience Award
- Professor Troy Van Voorhis was selected to be holder of the Paul M. Cook career development professorship
- Professor Gerald N. Wogan (Emeritus) received the Charles S. Mott Prize for Cancer Causation and Prevention

Building 18 Lobby Dedication

On December 15, 2004, following a luncheon in honor of the Dreyfus Foundation at the Faculty Club, representatives from the foundation were present at a dedication reception in the recently renovated lobby of Building 18. The renovation, which was made possible due to a generous grant from the Camille and Henry Dreyfus Foundation, is widely perceived as a very attractive and extremely functional addition to the Dreyfus Building. Representatives from the foundation who were present at the lobby dedication included Dorothy Dinsmoor, president; Mark J. Cardillo, executive director; Gerard Brandenstein, associate director; Harry Wasserman, board member, and Henry C. Walter, board member. The president of MIT, Dr. Susan Hockfield, the chancellor, Dr. Phillip Clay, the dean of Science, Dr. Robert Silbey, the architect of the new lobby, Roger Goldstein, members of Foundation Relations at MIT, and the Chemistry Department faculty were also among the guests. Dr. Silbey and Professor Lippard greeted and thanked the members of the Dreyfus Foundation, expressing deep appreciation for the many types of support the department has received from the foundation over the years.



L-R: Jack Oldham, director, MIT Foundation Relations; Dr. Mark J. Cardillo, executive director, Dreyfus Foundation; Professor Harry H. Wasserman, member, Board of Directors, Dreyfus Foundation; Henry C. Walter, treasurer and member, Board of Directors, Dreyfus Foundation; Dorothy Dinsmoor, president, Dreyfus Foundation; Gerard Brandenstein, associate director, Dreyfus Foundation; Janet Wasserstein, associate director, MIT Foundation Relations.

Named Speakers

The Department was pleased to welcome the following speakers during the year: Richard Zare, Stanford University, A. D. Little Lectures in Physical Chemistry, November 2004; Carolyn Bertozzi, University of California–Berkeley, T. Y. Shen Lectures in Biological Chemistry, December 2004; Andrew B. Holmes, University of Cambridge, Merck-Karl Pfister Lectures in Organic Chemistry, January 2005; Ben Cravatt, Scripps Research Institute, Novartis Lecture in Organic Chemistry, February 2005; Ronald Breslow, Columbia University, Buchi Lectures in Organic Chemistry, March 2005; Warren R. Roper, University of Auckland, A. D. Little Lectures in Inorganic Chemistry, April 2005; Hisashi Yamamoto, University of Chicago, Abbott Lecture in Organic Chemistry, May 2005; and Kendall N. Houk, University of California–Los Angeles, Bristol Myers Squibbs Lecture in Organic Chemistry, May 2005.



L-R: Steve Lippard, Carolyn Bertozzi, and T. Y. Shen.

On December 15, 2004, Dr. T. Y. Shen visited the department to hear Professor Carolyn Bertozzi give the T. Y. Shen Inaugural Lecture, “Chemistry in Living Systems: New Tools for Glycomics.”

Education

In the Fall of 2005, 41 students will enter the graduate program of the Chemistry Department. From September 2004 through June 2005, the department awarded 48 PhD degrees and 9 MS degrees. In the area of undergraduate education, 30 students graduated in June with BS degrees in chemistry. The 2004 Undergraduate Spring Awards Banquet was held on May 5, 2005, in The Hyatt Regency, Cambridge. The following awards were presented:

Alpha Chi Sigma Award for distinguished scholastic achievement, originality, and breadth of interest in chemistry: Torsak Luanphaisarnnont

Research Award for outstanding contributions in the area of research: Andrew Danford, Jillian Dempsey, and Karen C. O’Brien

Service Award for significant contributions in the area of service to the department: Stavroula Hatzios, Caroline Saouma, and Katherine Wu

Frederick D. Greene Teaching Award for outstanding contributions in the area of teaching: Jillian Dempsey

Merck Index Award for outstanding scholarship: Andrew Danford

CRC Freshman Chemistry Achievement Award for outstanding academic achievement in chemistry: Emily Tsui

Departmental Nomination for Association of MIT Alumnae (AMITA) Senior Academic Award: Jillian Dempsey

Hypercube Scholar Award for outstanding contributions to the advancement of computers in teaching: Kendra Bussey

American Institute of Chemists Foundation Award for outstanding achievement, ability, leadership, and character: Torsak Luanphaisarnmont

ACS Analytical Chemistry Award for an outstanding analytical chemist (junior year): Sarah Mahlstedt

Graduate Students Awards and Honors

- Kevin Anderson, Buchwald Group: 2005 Wyeth Scholar
- Julien Bachmann, Nocera Group: Morse Travel Grant; Bruker/MIT Symposium Poster Prize; David Johnson Fellowship
- Ghislaine Bailey, Swager Group: Best Poster Award at the Sixth International Symposium on Functional π Electron Systems
- Alexander Barnes, Griffin Group: National Science Foundation Graduate Research Fellowship
- Shin Grace Chou, Dresselhaus Group: Morse Travel Grant
- Elizabeth Colby, Jamison Group: NIH Postdoctoral Research Fellowship
- Josh Dunetz, Danheiser Group: Travel grant from the Cambridge Science Foundation
- Mary Elizabeth Farbman, Licht Group: Biotechnology Training Grant from MIT's BPEC program
- Josh Figueroa, Cummins Group: NIH Postdoctoral Fellowship; 8th Davison Prize for best inorganic thesis, July 1, 2004–June 30, 2005
- Hector Hernandez, Drennan Group: NIH Predoctoral Fellowship; Academic Resource Center UROP Graduate Mentor 2005; Student Advisory Group to the Corporation Committee on the Presidency; Vice President of the Graduate Student Council; Vice-Chair of the Student Advisory board to MIT's 16th President
- Javier Horta, Danheiser Group: 2005 Wyeth Scholar
- Amanda L. Kohnen, Danheiser Group: MIT Presidential Leventhal Fellowship; David Johnson Fellowship; American Council of Independent Laboratories Scholarship
- Maksym Kryvohuz, Cao Group: Lester Wolfe Fellowship
- Andrew M. Lauer, Jamison Group: National Science Foundation Graduate Research Fellowship
- Wan-Chen Lin, Licht Group: Lester Wolfe Fellowship
- Pia Lopez, Schrock Group: 7th Annual Northeastern Student Chemistry Research Conference "Graduate Women in Science Award for Best Poster Presentation"

- Chudi O. Ndubaku, Jamison Group, Hoffmann-La Roche Excellence in Chemistry Award
- Rebecca Nicodemus, Tokmakoff Group: National Science Foundation Graduate Research Fellowship; National Defense Science and Engineering Graduate Fellowship (accepted)
- Elizabeth Nolan, Lippard Group: Whitaker Health Science Fund Fellowship; National Young Investigator Award (Division of Inorganic Chemistry, ACS)
- Alison Ondrus, Movassaghi Group: Novartis Graduate Fellowship
- Jong-Ho Park, Molina Group: Scholarship from Kwanjeong Educational Foundation from Korea
- Steve Presse, Silbey Group: NSERC Doctoral Fellowship; Bourse de Doctorat FCAR; TA Award
- Peter Rye, Essigmann Group: 7th Annual Northeastern Student Chemistry Research Conference Best Poster Award
- Jennifer Schefiliti, Klibanov Group: Biotechnology Training Grant from MITs BPEC program
- Adam W. Smith, Tokmakoff Group: David A. Johnson Fellowship
- Eric R. Streiter, Buchwald Group: American Cancer Society Fellowship
- Marta Fernandez Suarez, Ting Group: La Caixa Foundation Fellowship
- Samuel Thomas, Swager Group: 2005 Wyeth Scholar
- Jessica Lynn Vey, Drennan Group: William Asbjornsen Albert Memorial Fellowship
- Elizabeth Vogel, Imperiali Group: 2005 Wyeth Scholar
- David Ward, Nelson Group: Finalist for the Truman Fellowship
- Katrina Woodin, Jamison Group: Donald O'Brien Fellowship

Research Highlights

Professor Mounji G. Bawendi's research group has continued progress in (1) the synthesis of new nanocrystal quantum dots, (2) the spectroscopy of quantum dots, (3) devices incorporating quantum dots, and (4) biomedical applications of quantum dots. His students have demonstrated new core shell quantum dots based on III-V semiconductors. They have used CdSe quantum dots to demonstrate photon bunching from biexcitons using single quantum dot spectroscopy. In collaboration with Professor Bulovic and Professor Kastner, they have demonstrated photoconductive and light emitting devices based on quantum dots, and finally, with collaborators at Massachusetts General and Beth Israel hospitals, they have demonstrated in vivo imaging applications of quantum dots.

The Catherine L. Drennan laboratory has solved the X-ray structure of hydroxypropylphosphonic acid epoxidase (HppE), an enzyme that catalyzes a novel epoxidation reaction in the synthesis of the antibiotic fosfomycin. The growing threat of antibiotic resistant microorganisms accentuates the importance of understanding the chemical mechanisms governing antibiotic biosynthesis. Our structural analysis of six states of HppE depicts conformational changes and binding events that accompany catalysis, painting a portrait of reactivity of this unusual enzyme (to be published online in *Nature* July 13, 2005).

In the Robert W. Field group, Dr. Hans Bechtel and Adam Steeves made progress toward their objective of using the Stark effect to detect HNC/HCN delocalized states in a bond-breaking isomerization. They constructed a discharge jet source of HNC and invented a new spectroscopic technique—polarization detected millimeter wave optical double resonance. Jeffrey Kay observed unexpected processes in the Rydberg spectrum of CaF and has shown them to be due to indirect coupling between Rydberg states mediated by the vibrational continuum of a single repulsive state. Robert Field will receive the 2006 Bomem-Michelson Award of the Coblentz Society.

During the past year, the Gregory C. Fu group has discovered the first method for achieving asymmetric cross-couplings of secondary alkyl electrophiles, using a chiral nickel catalyst. In addition, they have reported mechanistic studies that provide insight into palladium-catalyzed coupling reactions. Finally, they have described catalytic enantioselective methods for the generation of biologically active classes of molecules such as beta-lactones, arylpropionic acids, and nitriles.

The theme of the Timothy F. Jamison group's research is 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 provided to us by Nature, while others have their origins in unexpected products obtained in the course of other experiments. In the past year they developed several such chemical reactions, and they have enabled the synthesis of several complex molecules that may lead to new treatments for a variety of diseases, including cancer and AIDS.

Research accomplishments were reported by Professor Daniel S. Kemp and his coworkers. For more than forty years physical chemists and biophysicists have modeled the helix-coil equilibria of peptides in water under the assumption that stability is proportional to the number of residues within the helix. Using four different helicity measures they have disproved this assumption for the archetype case of polyalanines. The likely cause is hydrogen bonding cooperativity, long postulated by theorists but hitherto lacking an experimental example. Their result suggests a retuning of current folding algorithms.

The Stuart S. 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. In addition, they have synthesized artificial agonists that appear to assemble ion channels into functional clusters. These agonists will be used to investigate how supramolecular organization of synapses affects their function.

The Stephen J. Lippard laboratory demonstrated that DNA damaged by cisplatin—the drug used to cure the cyclist Lance Armstrong of testicular cancer—modifies the structure of the nucleosome, the building block of our chromosomes. Both the rotational setting and the translational positioning of platinated DNA on the core of histone proteins around which it wraps are affected. This phasing phenomenon may be central

to the recognition and processing of platinum damage in cancer cells treated with these drugs and possibly may be common to other DNA damaging events.

In the Mohammad Movassaghi group, the total synthesis of all tricyclic naturally occurring Myrmecarin alkaloids was accomplished. In the context of these studies, they developed a new palladium catalyzed N-vinylation of pyrroles and indoles. A new carbene-alcohol interaction was discovered and characterized both in the solution and in the solid state that led to the development of a catalytic amidation of esters using amino alcohols. They will continue their efforts toward the biomimetic total synthesis of complex alkaloids via cascade carbon-carbon bond forming reactions and the development of new synthetic methodologies.

Daniel G. Nocera studies the science of renewable energy at the molecular level. After the description of the first molecule to produce hydrogen photocatalytically from acidic solutions, research in the last year has succeeded in elucidating the photocatalytic process. Additionally synthesis of electron poor pac-man porphyrins has allowed us to perform photocatalytic oxygen atom transfer reactions while utilizing oxygen as the terminal oxidant on ever-more-difficult substrates, bringing us one step closer to the formation of O-O bonds.

The Jeffrey I. Steinfeld groups reports that reactive free radicals play an integral role in the chemical properties of the atmosphere. IntraCavity Laser Absorption Spectroscopy (ICLAS) is a powerful technique for identifying and measuring the concentration of reactive species. They have demonstrated that ICLAS is a feasible detection method for free radical species in a discharge flow tube. This implementation has been used to measure the rate of the reaction between atomic hydrogen and NO to form HNO in helium carrier gas. The sensitivity of ICLAS, coupled with the versatility of the discharge flow technique, suggests that intracavity spectroscopy will be a useful technique for kinetics measurements on free radicals and other reactive species.

In the Timothy M. Swager group, electronic polymer investigations have produced important advances in biosensory applications, including carbohydrate-functionalized polymers for trace detection of bacteria and amplified protease assays. He also recently reported a new general sensory concept based on attenuated lasing for explosives detection that adds a new level of sensitivity. The latter method can be applied to a wide range of systems.

Research in Alice Y. Ting's lab has focused on developing new protein labeling methodology and using this to image protein trafficking in living cells. They used the bacterial enzyme biotin ligase to catalyze site-specific conjugation of fluorophores, photoaffinity tags, and quantum dots to EGF receptors and AMPA-type glutamate receptors. The trafficking of these proteins was then imaged at the single-molecule level in living cells and neurons.

The Andrei Tokmakoff group is studying problems in solution-phase molecular dynamics. Their studies of liquid water probe the time scales and mechanism by which hydrogen bonds break and reform. Hydrogen bonds in water only break transiently

during fleeting collective rearrangements. Experimental protein-folding studies show how elements of the protein structure unfold sequentially during denaturing.

Timothy M. Swager
Department Head
John D. McArthur Professor

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