Department of Chemistry

In academic year 2016, the Department of Chemistry had 29.5 full-time faculty members, including eight assistant professors, two associate professors without tenure, and 19.5 full professors. There were two dual faculty appointments, one with the Department of Biological Engineering and one with the Institute for Medical Engineering and Science. Two faculty members (Alexander Klibanov and JoAnne Stubbe) had secondary appointments in Biology and Biological Engineering. Five additional faculty members (Arup Chakraborty, Catherine Drennan, Barbara Imperiali, Susan Solomon, and Steven Tannenbaum) had secondary appointments in Chemistry. In addition to research in biological, inorganic, organic, physical, and materials and nanoscience chemistry, the department continued its strong programs in undergraduate and graduate education, with 230 graduate students, 135 postdoctoral researchers, and 48 undergraduate chemistry majors.

On July 1, 2015, Professor Timothy F. Jamison assumed the position of head of the department. He inherited a strong and vibrant department from his predecessor, Professor Sylvia T. Ceyer, and proceeded to move forward with three promotions and three external hires in his first year. Professors Jeremiah Johnson and Bradley Pentelute were promoted to associate professor without tenure, and Professor Elizabeth Nolan was awarded tenure, all effective July 1, 2016. The department also hired Professor Alexander Radosevich, who joined the faculty from Pennsylvania State University as an associate professor without tenure, and Dr. Bin Zhang, who joined the faculty as an assistant professor, following a postdoctoral appointment at Rice University. Dr. Daniel Suess was also hired as an assistant professor, following a postdoctoral fellowship at the University of California, Davis, and will officially join the department next year.

In the fall of 2015, Professor Christopher C. Cummins was named the Henry Dreyfus Professor of Energy. In the spring of 2016, Professor Timothy F. Jamison was named the Robert R. Taylor Professor of Chemistry, Professor Matthew D. Shoulders was appointed to the Whitehead Career Development Professorship, and Professor Yogesh Surendranath was named the Paul M. Cook Career Development Professor.

Highlighted Faculty Awards and Honors

In July 2015, a special issue of *Advanced Synthesis & Catalysis* was dedicated to Professor Stephen L. Buchwald, the Camille Dreyfus Professor of Chemistry, in honor of his 60th birthday. The article's author, Eric N. Jacobsen, described Professor Buchwald as "one of the world's most famous and admired chemists, not only because of his outsized contributions to chemistry, but because of his larger-than-life personality."

In September 2016, Professor Buchwald was also named a William H. Nichols Medalist by the New York Section of the American Chemical Society (ACS). The Nichols Medal is the first gold medal for original chemical research and is given each year by the New York Section. It was established by William H. Nichols, a charter member of the American Chemical Society, in 1902. Since that year, 97 Nichols Medalists have been named, 16 of whom have gone on to receive the Nobel Prize in Chemistry.

In February 2016, Professor Buchwald was selected as the Gold Medal Lecturer and winner of the 22nd Nagoya Medal of Organic Chemistry. The Nagoya Gold Medal has been awarded every year, since its inception in 1995, to an organic chemist who has made significant original contributions to the field in its broadest sense.

In May 2016, Professor Arup Chakraborty, the Robert T. Haslam Professor of Chemical Engineering and director of MIT's Institute for Medical Engineering, was elected to the National Academy of Sciences (NAS) in recognition of his "distinguished and continuing achievements in original research."

In September 2015, Professor Mircea Dincă received the 2015 ExxonMobil Solid State Chemistry Faculty Fellowship. This fellowship recognizes young scientists who have made substantial contributions to the discipline of solid-state chemistry and have the potential to emerge as leaders in the field. In December 2015, Professor Dincă received the Polish Academy of Science's 2015 Dream Chemistry Award. This award, consisting of a statuette and a €15,000 prize, was established in 2013; it is given to a young scientist with a visionary research project in chemistry, combining chemistry with physics, biology, medicine, or materials engineering.

In April 2016, Professor Dincă was selected as the recipient of the National Science Foundation's 2016 Alan T. Waterman Award. This year marked the 40th anniversary of this prestigious prize, which is the National Science Foundation's highest honor recognizing an outstanding researcher under the age of 35.

In May 2016, Professor Dincă was selected by the Camille and Henry Dreyfus Foundation as one of its 2016 Camille Dreyfus Teacher-Scholars for his work, "Teaching Sponges New Tricks: Charge Transport and Heterogeneous Catalysis in Microporous Metal-Organic Frameworks." Since its inception in 1970, the Teacher-Scholar Awards Program has awarded more than $45,000,000 to support emerging young leaders in the chemical sciences.

In August 2015, Professor Robert Guy Griffin was awarded the 2016 E. Bright Wilson Award in Spectroscopy, sponsored by the ACS Division of Physical Chemistry. This prize recognizes outstanding accomplishments in fundamental or applied spectroscopy in chemistry. Professor Griffin was honored at an awards ceremony on March 15, 2016, in conjunction with the ACS national meeting in San Diego, CA.

In January 2016, Professor Jeremiah Johnson was named by the *Boston Globe*'s STAT News as one of "Three People to Watch in Kendall Square in 2016."

In March 2016, Stephen J. Lippard, the Arthur Amos Noyes Professor of Chemistry, was awarded the F.A. Cotton Medal for Excellence in Chemical Research. The medal is named for one of the most honored faculty members in Texas A&M University history, Dr. Albert Cotton. The medal is jointly awarded each year by the Texas A&M Department of Chemistry and the Texas A&M Section of the ACS. Dr. Cotton was widely considered to be one of the world's foremost inorganic chemists; he passed away on February 20, 2007.

In May 2016, Professor Lippard was one of four MIT faculty members to be elected to the prestigious American Philosophical Society. It was the first time in the society's history that four members from the same institution were elected. The four MIT researchers were among 33 new members elected to the society from academia, the arts, the professions, and public and private affairs.

In October 2015, Professor Elizabeth M. Nolan was named the recipient of the 2016 Eli Lilly Award in Biological Chemistry. This award, which was established in 1934 and is administered by the American Chemical Society's Division of Biological Chemistry, aims to stimulate fundamental research in biological chemistry by scientists under the age of 38. It honors "outstanding research of unusual merit and independence of thought and originality" and was presented to Professor Nolan in recognition of her contributions to metal homeostasis and human innate immunity.

In September 2015, Bradley L. Pentelute, the Pfizer-Laubach Career Development Assistant Professor, was selected as a recipient of the prestigious Novartis Early Career Award in Organic Chemistry. The company annually bestows this award upon two scientists who are "within 10 years of having established an independent academic research career in the areas of organic or bioorganic chemistry in the broadest sense."

In May 2016, Professor Pentelute was selected as one of four 2016 winners of the Amgen Young Investigators Award. This prize is given in recognition of young researchers whose scientific contributions significantly affect the field of drug discovery.

In November 2015, Professor Gabriela Schlau-Cohen was awarded the Smith Family Award for Excellence in Biomedical Research. This award, which consists of a $300,000 prize, aims to support promising junior faculty members who are beginning to establish their own laboratories and research programs with a focus on basic biomedical science.

In August 2015, Alex K. Shalek, the Hermann L. F. von Helmholtz Career Development Assistant Professor of Health Sciences and Technology, was awarded a 2015 Beckman Young Investigator Award. The Beckman Young Investigator award is intended to provide research support to the most promising young faculty members in the early stages of academic careers in the chemical and life sciences, particularly to foster the invention of methods, instruments, and materials that will open up new avenues of research in science. In October 2015, Professor Shalek received a National Institutes of Health (NIH) New Innovator Award. The New Innovator Award, established in 2007, supports unusually innovative research from early-career investigators who are within 10 years of their terminal degree or clinical residency and have not yet received a research project grant or equivalent NIH grant.

In October 2015, Matthew D. Shoulders, the Whitehead Career Development Professor, received an NIH New Innovator Award. The New Innovator Award, established in 2007, supports unusually innovative research from early-career investigators who are within 10 years of their terminal degree or clinical residency and have not yet received a research project grant (R01) or equivalent NIH grant.

In February 2016, Timothy M. Swager, the John D. MacArthur Professor of Chemistry, was selected to receive the 2016 Gustavus John Esselen Award for Chemistry in the Public Interest. This award, which annually recognizes a chemist "whose scientific and technical work has contributed to the public well-being," is one of the most prestigious honors provided by the Northeastern Section of the ACS.

In February 2016, Yogesh Surendranath, the Paul M. Cook Career Development Professor, received a Sloan Research Fellowship from the Alfred P. Sloan Foundation. Awarded annually since 1955, Sloan Research Fellowships are given to early-career scientists and scholars whose achievements and potential identify them as rising stars among the next generation of scientific leaders.

Development News—Major Gifts During Academic Year 2016

Dr. Scott Rocklage, PhD '82, and his wife Patty completed their pledge of $250,000 to assist with the costs associated with the renovation of nanochemistry and nanotechnology laboratory space in Building 2. Dr. Rocklage carried out his PhD studies in the Department of Chemistry under Professor Richard R. Schrock, who won the Nobel Prize in Chemistry. A event to thank and celebrate the Rocklages for their gift will be held on July 18, 2016.

Dr. Judith E. Selwyn, PhD '71, and her husband, Dr. Lee L. Selwyn, PhD '69, as trustees of the Lee L. and Judith E. Selwyn Foundation, pledged a further $250,000. This gift brings their total pledge to $500,000 to support the new Chemistry undergraduate teaching laboratories that will be housed in the MIT.nano building, which is due to be completed in 2018.

Dr. Jan Krouwer, PhD '73, and his wife, Ruby, established the Jan S. and Ruby S. Krouwer endowed fund to support graduate students in the Department of Chemistry. Jan, a native of New York, earned his BS from Tufts University, followed by a PhD in synthetic organic chemistry in the Department of Chemistry at MIT under the late Professor Glenn Berchtold.

To coincide with a 60th birthday symposium in his honor, Stephen L. Buchwald, the Camille Dreyfus Professor of Chemistry and associate head of the department, and his wife Susan Haber established the Buchwald-Haber Family Fund with a gift of $100,000 and a further pledge of $150,000. The Buchwald-Haber Family Fund is an endowed fund to support graduate students, with a preference for those who are studying organic chemistry.

The department is extremely grateful to the following alumni and friends for their support by way of endowed and expendable summer graduate student support (and, in some cases, half-yearly support). The department is also very grateful to those who give travel grants for students to attend national and international meetings and conferences throughout the year:

Dr. Ping S. Chu

Dr. Michael E. Strem

Professor Alan Davison

Mrs. Merece Johnson

Dr. David L. Morse (Morse Travel Fund)

Dr. Daniel C. Harris and his wife Mrs. Sally L. Harris

Ms. Judith E. Hughes and her sister, Ms. Mary Lee Berger-Hughes

Dr. Kin Chun T. Luk and his wife Mrs. Yuen-Kwan Luk

Professor Jeffrey I. Steinfeld

Dr. and Mrs. T-Y Shen

Dr. Gregory C. Fu (Fu Travel Fund)

Alumni and Friends Reception

On March 31, the Department of Chemistry held an Alumni and Friends Reception in the Pappalardo Room. Two assistant professors, Brad Pentelute and Yogi Surendranath, presented their research to an appreciative audience. After the talks, Professor Jamison invited guests to ask questions and a lively exchange ensued. Members from the professors' research groups also attended and enjoyed the opportunity to share details of their current work and future aspirations. As he expressed gratitude to the department donors present, Professor Jamison also encouraged all to consider the department's need to increase graduate fellowship support. "The department's risk of losing its competitive edge to other institutions who can offer more attractive financial packages is a critical concern," he said. He noted that in MIT's soon-to-be launched comprehensive campaign, graduate student fellowship support will be listed as a core need for the Institute.

Named Lectures

The department welcomed the following named speakers during the fall of 2015 and spring of 2016:

Sigma-Aldrich Lecture in Organic Chemistry: Guangbin Dong, University of Texas, Austin

Boehringer-Ingelheim Lecture in Organic Chemistry: M. Christina White, University of Illinois, and Carl Busacca, Boehringer-Ingelheim

Merck-Banyu Lecture in Organic Chemistry: Jun Takaya, Tokyo Institute of Technology

MIT-Merck Lecture in Organic Chemistry: Kendall N. Houk, University of California, Los Angeles, and Jingjun Yin, Merck

Georgia-Pacific Lecture in Organic Chemistry: Luis M. Campos, Columbia University

Buchi Lecture in Organic Chemistry: Dirk Trauner, Ludwig Maximilian University of Munich

A.D. Little Lecture in Physical Chemistry: Professor R. J. Dwayne Miller, University of Toronto

Davison Lecture in Inorganic Chemistry: Anthony Cheetham, University of Cambridge

TY Shen Lectures in Biological Chemistry: Suzanne Walker, Harvard University

Organic Syntheses Lectures in Organic Chemistry: Mark Lautens, University of Toronto, and Thomas R. Hoye, University of Minnesota

Novartis Lectures in Organic Chemistry: Steven V. Ley, University of Cambridge, and Kian Tan, Novartis

Bristol-Myers Squibb Lecture in Organic Chemistry: Joseph M. Fox, University of Delaw are, and Chris Stouggatakis, Bristol-Myers Squibb

Chemistry in Industry Lecture: John Gavenonis, DuPont

Pfizer-MIT Lecture in Organic Chemistry: Nicola Pohl, Indiana University

Chemistry in Industry Lecture: Jotham Coe, Pfizer

Serving the Institute

The Department of Chemistry provides key educational services to the Institute. During academic year 2016, the Department of Chemistry taught 1,453 MIT undergraduate students in the areas of biochemistry, inorganic, organic, and physical chemistry. The department was also the home for 51 students from the Undergraduate Research Opportunities Program, which provides important mentoring relationships for students from a number of departments, including Chemistry, Biology, Mathematics, Physics, Chemical Engineering, Biological Engineering, Mechanical Engineering, and Materials Science and Engineering.

Chemistry Majors

The Department of Chemistry continues to attract a very talented group of undergraduates, with a total of 48 majors across the three years. This year, 16 students received SB degrees in chemistry. On the basis of self-reported data, 44% of the Class of 2016 is bound for graduate school (including MD/PhD programs); 12% of the class plans to attend medical school; 25% will seek employment, and 19% were unknown or undecided as of Commencement.

Undergraduate Research Opportunities Program

The Undergraduate Research Opportunities Program continues to be the capstone experience for the department's undergraduates. More than 94% of the Class of 2016 worked in a research group at least once during their degree program. Looking at the Class of 2017 and Class of 2018, so far almost 75% have worked in a research group at least once. Chemistry's undergraduates have the unique opportunity to conduct research alongside faculty, postdoctoral associates, and graduate students.

Chemistry Teaching Assistants

Chemistry's graduate student teaching assistants are some of the best at MIT. This year, students scored 75% of the department's TAs at 6.0 or higher on a 7.0 scale. Of those, 57% scored a 6.5 or higher.

Undergraduate Awards

Undergraduate awards were given out at the Undergraduate Recognition Banquet on May 12, 2016.

Freshmen Chemistry Achievement Award, for outstanding academic achievement in chemistry

Songela Chen

Christopher Hillenbrand

Outstanding Sophomore Achievement Award, for outstanding achievement in academics, research, and service to the Department of Chemistry

David Vaccaro

ACS Analytical Chemistry Award, for outstanding achievement by a junior in experimental chemistry

James Deng

Outstanding UROP Presentation Award, for outstanding undergraduate research and in recognition of the best presentation at the 2016 Chemistry UROP Symposium

Emma Chant

Alpha Chi Sigma Award, for outstanding achievement in scholarship, research, and service to the Department of Chemistry

Lily Chen

Diptarka Hait

Research Award, for outstanding contributions in the area of research

Hope Flaxman

Julia Page

Reuben Saunders

Tanyaporn Pattarabanjird

Frederick D. Greene Teaching Award, for outstanding contributions in the area of teaching

Diptarka Hait

Ilana Porter

ACS Inorganic Chemistry Award, for excellence in inorganic chemistry

Sarah Alexander

Merck Index Award, for outstanding scholarship

Sarah Alexander

Hope Flaxman

Julia Page

Reuben Saunders

Service Award, for significant contributions in the area of service to the Department of Chemistry

Natalie Burgos

Alyssa Napier
Tanyaporn Pattarabanjird
John Read

Hypercube Scholar Award, for outstanding contribution to the advancement of computers in teaching

Ilana Porter

Special Recognition, Association of MIT Alumnae Award Nominee

Hope Flaxman

Phi Beta Kappa 2016 Inductees

Sarah Alexander
Lily Chen
I-Ling Chiang
Hope Flaxman
Diptarka Hait
Julia Page
Ilana Porter
Reuben Saunders

Teaching Assistant Awards

Lindsey Backman
Lisa Cunden
Joseph Dennis
Krysta Dummit
Michael Geeson
Corey Kaminsky
Ryan King
Richard Liu
Alexander Loftis
Nicole Moody
Zachary Nelson
Cole Perkinson
Katherine Shulenberger
Tho Tran
Jason Yoo
Frieda Zhang

Additionally, Alyssa Antropow will receive the Department of Chemistry Award for Continued Excellence in Teaching for academic year 2016.

Excerpts from TA Evaluations

She was an amazing TA. She always went above and beyond to make sure students knew what was going on and made chemistry interesting. She constantly gave us encouragement.

Her handouts are gold. She really cared about our success and tried to help us learn.

[NAME] was great in every way in the lab. He always looked out for every single student in his group, providing tips and assistance.

She's great, she's funny, super interested in what she's teaching, and good at teaching.

[NAME] has been one of my best TAs here at MIT. He is very knowledgeable on the material and does a very good job of explaining it. He reviews the important topics during recitation, and goes over common mistakes. He is very experienced. He is also accessible and available for his students to answer questions.

Thanks for making recitation relatively fun. I think it was good that you asked a lot of questions and waited until someone would venture an answer. The material you covered was always relevant and deepened understanding of the concepts. Recitation really helped me prepare for exams, particularly because of the more challenging/special case problems we covered.

The best TA I've had. Very impressive with her ability to teach the concepts. Wish she could TA for all my classes!!!

[NAME] was an amazing TA. He had the class very well organized and was genuinely interested in us learning the material. He also took the time during down time to ask us about where we were headed in life and was genuinely interested and able to provide good advice. He was a pleasure to have as a TA.

[NAME] was super excited about this class, the lab was very well organized, and he was more than willing to spend a long time in office hours making sure that we truly understood the material.

Doctoral and Master's Degree Recipients

Date	Name	Degree	Group
Sep-15	Andrew Beyler	PhD	Bawendi
Sep-15	Thomas Bischof	PhD	Bawendi
Sep-15	James Colombe	PhD	Buchwald
Sep-15	Philip Hamzik	PhD	Danheiser
Sep-15	Olesya Haze	PhD	Swager
Sep-15	Hyangsoo Jeong	PhD	Schrock
Sep-15	Minyuan Li	PhD	Dincă
Sep-15	Vinita Lukose	PhD	Imperiali
Sep-15	Mikael Minier	PhD	Lippard

Date	Name	Degree	Group
Sep-15	Lisa Olshansky	PhD	Nocera
Sep-15	Nathaniel Park	PhD	Buchwald
Sep-15	Ishan Patel	PhD	Tidor
Sep-15	Amy Rabideau	PhD	Pentelute
Sep-15	D.W. Rowlands	SM	Ceyer
Sep-15	Ye Tao	PhD	Degen
Sep-15	Sarah Tasker	PhD	Jamison
Sep-15	Yu-Pu Wang	PhD	Danheiser
Sep-15	Yifeng Wei	PhD	Stubbe
Sep-15	Yang Yang	PhD	Buchwald
Feb-16	Darin Bellisario	PhD	Strano
Feb-16	Syuan-Ming Guo	PhD	Bathe
Feb-16	Tamara Halkina	PhD	Jamison
Feb-16	Ryan Palmer	SM	Van Humbeck
Feb-16	Tuo Wang	PhD	Hong
Feb-16	Zackary Wong	SM	Buchwald
Jun-16	Joseph Azzarelli	PhD	Swager
Jun-16	Phoom Chairatana	PhD	Nolan
Jun-16	Hang Chen	PhD	Chakraborty
Jun-16	Haritha Reddy Chileveru	PhD	Nolan
Jun-16	Luigi De Marco	PhD	Tokmakoff
Jun-16	Joseph Azzarelli	PhD	Swager
Jun-16	Joseph Elias	PhD	Shao-Horn
Jun-16	Owen Fenton	PhD	Anderson
Jun-16	Gregory Guitierrez	PhD	Swager
Jun-16	Gihan Hewage	SM	Johnson
Jun-16	Victoria Hung	PhD	Ting
Jun-16	Michael Huynh	PhD	Nocera
Jun-16	Hongik Hwang	PhD	Xu
Jun-16	Stephanie Lam	PhD	Ting
Jun-16	Sophie Liu	PhD	Swager
Jun-16	Huai Jin Ken Le Loh	PhD	Ting
Jun-16	Michael Mavros	PhD	Van Voorhis
Jun-16	Anna Jolene Mork	PhD	Tisdale
Jun-16	Benjamin Ofori-Okai	PhD	Nelson
Jun-16	Kanchana Ravichandran	PhD	Stubbe
Jun-16	Michael Reppert	PhD	Tokmakoff
Jun-16	Paula Ruiz-Castillo	ScD	Buchwald
Jun-16	Jennifer Scherer	PhD	Bawendi
Jun-16	Colby Steiner	PhD	Nelson
Jun-16	Samuel Teitelbaum	PhD	Nelson
Jun-16	Peter Thill	PhD	Chakraborty

Date	Name	Degree	Group
Jun-16	David Veysset	PhD	Nelson
Jun-16	Matthew Welborn	PhD	Van Voorhis
Jun-16	Aleksandr Zhukhovitskiy	PhD	Johnson

A photo gallery of the Hooding Reception, held on June 2, 2016, is available, as is a photo gallery of the Commencement Reception, held on June 3, 2016, featuring the department's seniors.

Faculty Research Highlights

Stephen L. Buchwald

In the past year, the Buchwald research group has made several notable contributions in the field of synthetic methodology for the formation of carbon–carbon and carbon–heteroatom bonds. In particular, the design of new ligands has facilitated the palladium-catalyzed mild fluorination of aryl halides and the arylation of hindered amines. The development of palladium-mediated reactions has also enabled the modification of complex biomolecules. Additionally, the Buchwald group has reported a variety of copper-hydride catalyzed methods that allow for the highly selective construction of enantiomerically pure carbon–carbon and carbon–nitrogen bonds. The techniques developed are general, practical, and commonly used for the discovery, development, and manufacturing of pharmaceutical drugs and materials.

Jianshu Cao

Biological systems have evolved over millions of years to form perfect structures for executing complex functions, such as photosynthesis, gene regulation, and immune responses to infectious diseases. The Cao group is interested in elucidating the structure–function relationship in biological machines and in exploring this relationship for the optical design of artificial systems useful for solar energy conversion, biomechanics, and quantum technology. In this pursuit, researchers in the Cao laboratory have discovered emerging new features of physical laws when they are applied to nano-scale, non-equilibrium, and highly structured systems.

Sylvia T. Ceyer

The Ceyer group has continued its investigation into the non-equilibrium effects of multiple collisions in the etching of silicon. These results will yield a fundamental dynamical principle that is applicable to the development of more efficient reactivity at interfaces of covalent solids. Researchers have also discovered a low-energy pathway for the dissolution of hydrogen into the bulk of nickel that is enabled by the formation of a gold–nickel alloy on the surface. This alloy is an excellent model for the Raney nickel alloy, used commercially in all heterogeneous catalytic hydrogenation reactions.

Arup K. Chakraborty

The Chakraborty group continued its efforts to understand the mechanistic basis of how a specific and systemic immune response to a pathogen occurs, and how its aberrant

regulation leads to disease. Research aimed toward understanding how this knowledge can be harnessed for the rational design of vaccines and therapies is also an important facet of the laboratory's work. Chakraborty also serves as the director of the Institute for Medical Engineering and Science, taught a core Chemical Engineering graduate subject, and, with Tyler Jacks, coordinated the crafting of the campaign White Paper on Health. He was elected to the NAS this year, making him probably the first person to be elected to the NAS and the National Academy of Engineering for completely different bodies of work recognized by completely different communities of researchers. He continues to serve as a member of the US Defense Science Board and as a senior editor of *eLife*, one of the premier journals in biology.

Christopher C. Cummins

The Cummins laboratory reported the synthesis, isolation, and detailed characterization of a salt containing the diphosphatriazolate ion, $P_2N_3^-$, a planar cyclic five-membered ring anion composed entirely of phosphorus and nitrogen. The remarkable stability of this ion was shown to have electronic origins of aromaticity, a stabilizing factor normally found in the domain of planar organic hydrocarbons having delocalized pi-systems, of which the prototype is the benzene molecule. The synthesis of $P_2N_3^-$ was achieved via P_2 transfer from a molecular precursor. Researchers also synthesized and reported molecular precursors to other small molecules, including HCP, which was characterized in the gas phase by microwave spectroscopy and laser-induced fluorescence. In another project, it was shown that a variety of anionic metaphosphate acids could be prepared with organic cations imparting solubility in polar organic media for a variety of applications in battery, catalyst, and coordination chemistry research.

Rick L. Danheiser

One of the main accomplishments of the Danheiser laboratory during the past year was the extension of researchers' so-called tandem benzannulation/heterocyclization strategy to include several new classes of heteroaromatic compounds. This strategy for chemical synthesis provides efficient access to important types of organic compounds that have applications in biology and medicine.

Mircea Dinca

In one major advance, the Dincă group produced the best solid catalyst for ethylene dimerization, a large industrial process that no other solid could catalyze effectively before. Using similar custom porous materials, researchers produced the world's first noncarbon electrochemical double layer capacitor, a rapid-charging energy storage device. Dincă was selected for the Alan T. Waterman Award, the NSF's most prestigious award for scientists and engineers under 35.

Catherine L. Drennan

A major finding in the Drennan laboratory in 2015–2016 was that oil bacteria protect themselves from light by making carotenoids, the orange pigment found in carrots, but need to make these pigments only in the presence of light. They use a light-sensing molecule, vitamin B_{12}, bound to a protein called CarH ("Car" for carotenoid), to sense light and turn on carotenoid production. In the past year, the Drennan laboratory

published in *Nature* crystallographic snapshots of CarH in both light and dark states to visualize how this regulation works at a molecular level. These structures are the first of a B_{12}-dependent light sensor.

John M. Essigmann

The Essigmann laboratory published its finding that 5-chlorocytosine, a derivative of the normal DNA base cytosine, causes C to T mutations in living cells. This modified base forms when DNA, or nucleotides in the pool of raw material used to synthesize DNA, is oxidized by macrophages and other cells of the innate immune system. The type of mutation seen is the principal one found in cells that have experienced carcinogenic inflammation.

Robert W. Field

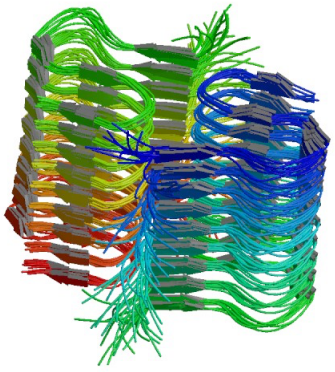
Vinylidene is an unstable isomer of acetylene that is widely believed to live for less than a picosecond. The Field group is preparing to observe the J = 0 to 1 rotational spectrum of vinylidene at 50 kHz resolution. What happened to the uncertainty principle? The researchers showed that an electronically excited state of SO_2 has unequal S–O bond lengths. Although it is true, this is an insult to chemical intuition. The energy level pattern reveals that this unexpected structure is caused by a "vibronic" interaction with two higher-energy electronic states; it also determines the equilibrium structures of these states.

Robert Guy Griffin

The Griffin laboratory solved the first complete atomic resolution structure of Abeta 1-42, the protein that is believed to be the toxic species in Alzheimer's disease, using magic-angle spinning nuclear magnetic resonance imaging (Figure 1). The research group also developed a new class of time domain experiments—NOVEL, ramped NOVEL, and integrated solid effect—for dynamic nuclear polarization that circumvents the inverse field dependence of continuous wave experiments.

Mei Hong

The Hong research group investigated the structure and dynamics of an early-onset Alzheimer's Abeta mutant, the Arctic Abeta, and elucidated the zinc coordination structure of a catalytic amyloid fibril. In addition, they investigated both the influenza B virus M2 protein's structure and proton-conduction equilibria and structural polymorphism of cellulose microfibrils in plants. Finally, Mei and her researchers determined the conformation of a viral fusion protein in lipid membrane and how the protein induces membrane curvature.



Atomic Resolution Structure of Monomorphic Aβ42 Amyloid Fibril

Timothy F. Jamison

In collaboration with Klavs F. Jensen (Chemical Engineering), the Jamison group developed the first chemical synthesis platform, which features plug-and-play operation and automated reaction optimization. Also in collaboration with Klavs F. Jensen, as well as Allan Myerson (Chemical Engineering), the group developed a plug-and-play, refrigerator-sized system capable of end-to-end continuous manufacturing of pharmaceutical substances. Potential applications include disaster relief, developing nations, green manufacturing, and orphan and neglected diseases. Another accomplishment of the Jamison laboratory was the development of a novel photoredox catalytic system under flow conditions to generate alpha-amino acids via the coupling of amines and carbon dioxide.

Jeremiah A. Johnson

The Johnson laboratory developed new strategies for the synthesis of polymers with precise molecular structure, a new visible-light-induced organocatalyzed polymerization reaction, and a class of polymer metal-organic-cage gel materials that display unprecedented mechanical properties.

Stephen J. Lippard

The Lippard laboratory prepared the first platinum drug candidate with immune checkpoint blockade properties, and identified the protein HMGB4 in testicular germ cell tumors that sensitizes them to cisplatin, consistent with shielding of platinum-DNA adducts from excision repair. With the help of various collaborators, they also discovered a major role for mobile zinc ions in learning, memory, and sensory perception (olfaction, audition, vision) in the brain.

Mohammad Movassaghi

The Movassaghi laboratory continues to focus on the development of new strategies and technologies for complex molecule synthesis. They recently reported concise and unified total syntheses of (+)-asperazine and (+)-pestalazine A and revised the molecular structure of (+)-pestalazine A. Additionally, they reported the most complex application of the laboratory's diazene-based strategy for complex fragment assembly in the context of researchers' biogenetically inspired total synthesis of (–)-communesin F, providing the most concise synthesis of this potent antiproliferative alkaloid. The hallmark of the laboratory's syntheses is their unparalleled efficiency and high level of stereochemical control in complex settings, taking full advantage of the inherent chemistry of plausible biosynthetic intermediates.

Keith A. Nelson

This year, the Nelson laboratory used its recently developed strong-field terahertz (THz) frequency pulses to induce the emission of visible light (a 100-times increase in photon energy) from quantum dot electroluminescence and to shift the quantum dot absorption spectrum across the entire visible spectrum. The result enables novel THz

sensors and THz frequency electro-optic modulators. This and other nonlinear effects that the researchers have demonstrated rely on the THz-frequency electric field. The Nelson laboratory also used the THz magnetic field to extend two-dimensional electron spin resonance to the THz-frequency range, with wide-ranging applications in the study of molecular and conventional magnetism and high-spin transition metal molecular and biomolecular complexes.

Elizabeth M. Nolan

The Nolan laboratory demonstrated that the human host-defense protein S100A12 inhibits the growth of pathogenic fungi and utilizes Ca(II) ions to enhance both its antifungal activity and Zn(II)-binding ability. In studies of the metal-chelating host-defense protein human calprotectin, the laboratory discovered that Ca(II) binding shields the protein scaffold from attack by host and bacterial proteases. In collaboration with Professor Michael Neidig at the University of Rochester, magnetic circular dichroism spectroscopic studies of Fe(II)-bound human calprotectin were performed. These revealed details about the Fe(II)-binding sites and electronic structure of this metal-sequestering host-defense protein.

Bradley L. Pentelute

Throughout evolution, nature has developed molecular machines to rapidly manufacture, tailor, and deliver large functional biopolymers, such as proteins, into specific cells. Inspired by these mechanisms of nature, over the past year, the Pentelute laboratory has worked to invent new chemistry for the efficient and selective modification of proteins, to “hijack” these biological machines for efficient drug delivery into cells, and to create new machines to rapidly and efficiently manufacture peptides and proteins.

Gabriela S. Schlau-Cohen

In its first full year, the Schlau-Cohen laboratory identified the protein conformational dynamics and mechanisms responsible for photoprotection under high-light conditions in moss and algae. They also constructed a single-molecule microscope that is an order of magnitude more stable than traditional single-molecule microscopes. Finally, they produced model membrane-protein systems containing bacterial photosynthetic light-harvesting complexes.

Richard R. Schrock

In academic year 2016, the Schrock laboratory has discovered how to employ electron-poor olefins, such as dichloroethylene and 1,1,1,3,3,3-hexafluoro-2-butene, in olefin metathesis reactions. This discovery should dramatically expand the possible applications of olefin metathesis to the synthesis of complex organic molecules. They have also prepared a molybdenum catalyst for the reduction of molecular nitrogen with protons and electrons that is stable to protons, thereby bringing closer a practical synthesis of ammonia from protons and electrons that avoids the production of carbon dioxide on a large scale—a current drawback of the Haber-Bosch process.

Alex K. Shalek

This year, in collaboration with the Love laboratory (Chemical Engineering), the Shalek Laboratory co-developed an ultra-high-throughput, low-cost, microwell-based single-cell RNA-Seq platform called Seq-Well. This technology relies on the co-confinement of uniquely barcoded mRNA capture beads and individual cells using a polydimethylsiloxane microwell array, and allows simultaneous analysis of mRNA transcripts from thousands of individual cells while still retaining each transcript's cell of origin. Relative to previous embodiments, Seq-Well can be applied to many samples at once (using multiple devices), works with as few as 500 cells (because of the elimination of most upstream processing steps), and is portable (complex peripherals are not needed), making it ideally suited to profiling complex biological specimens in both basic and clinical research settings. Shalek envisions that Seq-Well will inform an era of precision medicine, accelerating biological discovery by enabling routine and cost-effective transcriptional profiling of clinical samples at single-cell resolution. Toward realizing this goal, in collaboration with several researchers, the Shalek laboratory has begun investigating the composition of multiple tissues and clinical samples, including tumor resections, gut pinch biopsies, female genital tract cytobrushes from HIV patients, and TB-infected bronchial alveolar lavages.

Matthew D. Shoulders

The Shoulders laboratory developed a chemical genetic method that allows control of the levels of any endogenous mRNA transcript across a three-orders-of-magnitude dynamic range in human cells using a small molecule. They also delineated exactly how remodeling the cellular protein folding environment resolves collagen secretion defects involved in osteogenesis imperfecta. Other highlights included invention of the first highly selective method for inhibiting heat shock factor 1—a protein important in cancer and neurodegenerative disorders.

Yogesh Surendranath

In academic year 2016, the Surendranath laboratory developed a new class of molecularly precise heterogeneous catalysts based on inexpensive graphite, uncovered the mechanistic basis for the selective conversion of carbon dioxide to fuel using renewable energy, and developed a new class of tunable porous catalysts for carbon dioxide to fuels conversion.

Timothy M. Swager

The Swager research group developed new materials for wearable sensors that can be inductively powered and read by a smartphone and that can detect chemical threats at parts-per-billion levels. This revolutionary technology enables new generations of sensors for occupational safety and can be used to protect soldiers and first responders from chemical threats.

Jeffrey Van Humbeck

Over the past year, the Van Humbeck laboratory discovered a copper-based catalyst that has the ability to selectively bind to nitrogen-containing heterocycles and direct reactions to carbon–hydrogen bonds nearby, even in the presence of inherently more

reactive carbon–hydrogen bonds elsewhere in the reaction mixture. This approach has been demonstrated in reactions that have value for creating biologically active small molecules, such as amination and oxidation. Additional reactions of high value in pharmaceutical chemistry were discovered by combining palladium catalysts with chiral Lewis acids.

Troy Van Voorhis

In the past year, the Van Voorhis research group has shifted to focus more on organic light-emitting diodes, compared with previous work on organic photovoltaics. In particular, they have worked on designing molecules for thermally activated delayed fluorescence and the dynamics of electrons and holes in these devices. They have also begun developing fragment-based methods in electronic structure theory.

Adam Willard

The Willard research group developed a new theoretical model for simulating magnetic field effects in charge transfer dynamics. The microscopic electronic processes that mediate photocurrent generation in organic photovoltaics are difficult to probe experimentally. These processes involve particles with spin and thus are sensitive to the presence of a magnetic field. This sensitivity encodes important microscopic information that is otherwise unattainable. This model has allowed the Willard group, for the first time, to extract this information from experiments.

Timothy F. Jamison
Department Head
Robert R. Taylor Professor of Chemistry