Department of Chemistry

In academic year 2016–2017, the Department of Chemistry had 29.5 full-time faculty (including two dual faculty appointments, one with the Department of Biological Engineering and one with the Institute of Medical Engineering and Science): seven assistant professors, three associate professors without tenure, two associate professors with tenure, and 17.5 full professors. One faculty member (Alexander Klibanov) has a secondary appointment in Biological Engineering. Five additional faculty members (Arup Chakraborty, Catherine Drennan, Barbara Imperiali, Susan Solomon, and Steven Tannenbaum) have secondary appointments in Chemistry. Professor JoAnne Stubbe retired from teaching in the summer of 2016, and Professor Alice Ting left the department. In addition to research in biological, inorganic, organic, materials and nanoscience, and physical chemistry, the department continued its strong programs in undergraduate and graduate education with 230 graduate students, 135 postdoctoral researchers, and 48 undergraduate chemistry majors.

Professor Elizabeth Nolan was awarded tenure effective July 1, 2016, and Professor Jeremiah Johnson was awarded tenure effective January 16, 2017. In July 2016, Bin Zhang joined the department following a postdoctoral appointment at Rice University. The department also welcomed Professor Alexander T. Radosevich, who joined the faculty from Pennsylvania State University in summer 2016.

In spring 2017, Professor Gabriela Schlau-Cohen was appointed to the Cabot Career Development Professorship, and Professor Alex K. Shalek was appointed to the Pfizer-Laubach Professorship.

Faculty Awards and Honors

In January 2017, Moungi Bawendi, the Lester Wolfe Professor of Chemistry, was selected by the prize committee of the World Technology Awards to receive the award in the materials category for his work in semiconductor nanocrystals, also known as quantum dots.

In March 2017, Stephen L. Buchwald, the Camille Dreyfus Professor of Chemistry, received the Carothers Award from the Delaware section of the American Chemical Society (ACS). The award, given annually, honors scientific innovators who have made outstanding contributions to and advances in industrial applications of chemistry.

Professor Christopher C. Cummins, the Henry Dreyfus Professor of Chemistry, was elected to the National Academy of Sciences in May 2017 in recognition of his "distinguished and continuing achievements in original research." Professor Cummins was one of six MIT faculty members elected in 2017. In June, Professor Cummins was named the 2017 awardee of the Linus Pauling Medal in recognition of his unparalleled synthetic and mechanistic studies of early-transition metal complexes, including exploratory methods of development to improve nitrogen and phosphorous utilization.

Professor Rick Lane Danheiser, the A.C. Cope Professor of Chemistry, was one of 65 members of the American Chemical Society to be named a 2017 ACS Fellow. ACS lauded Professor Danheiser's numerous innovative and elegant methodologies, including the Danheiser annulation, the Danheiser benzannulation, and cyclo-additions of highly unsaturated conjugated molecules for the synthesis of complex carbocyclic and heterocyclic organic compounds.

In May 2017, Professor Mircea Dincă was awarded one of 10 early-stage energy research seed fund grants (each in the amount of $150,000) for his project "Designer Electrocatalysts for Energy Conversion: Catalytic O2 Reduction, CO2 Reduction, and CH4 Activation with Conductive Metal-Organic Frameworks." Professor Dincă's project, a collaboration with Professor Evelyn Wang of the Department of Mechanical Engineering, aims to develop a new technology that can be used to harvest water in even the most arid regions of the globe. Using a metal-organic framework, Dincă and Wang will create a passive solar device that can extract clean, fresh water from the air at any range of humidity. The seed funds for the project will support the development of metal-organic frameworks that can be used for providing water to remote areas with greatly reduced infrastructure costs.

Professor Robert Guy Griffin was awarded the 2017 Richard R. Ernst Prize in Magnetic Resonance. The prize recognizes groundbreaking applications of new or previously known techniques in all areas of magnetic resonance.

In December 2016, Professor Stephen J. Lippard, the Arthur Amos Noyes Professor of Chemistry, was unanimously selected by the American Institute of Chemists (AIC) Awards Committee to receive the AIC Gold Medal (the institute's highest award). Professor Lippard was chosen to receive this illustrious prize due to his groundbreaking research and his extensive service to the profession of chemistry. In addition, in September 2016, the Welch Foundation named Professor Lippard co-winner of the Robert A. Welch Award in Chemistry. This award is given annually to foster and encourage basic chemical research and to recognize the value of chemical research contributions for the benefit of humankind.

Professor Keith A. Nelson, the Haslam and Dewey Professor of Chemistry, was named the 2017 recipient of the Bomem-Michelson Award. The award is dedicated to the memory of Professor A.A. Michelson, developer of the Michelson interferometer. ABB sponsors the award to honor scientists who have advanced vibrational, molecular, Raman, or electronic spectroscopy techniques.

In January 2017, Professor Elizabeth M. Nolan was one of 102 scientists and researchers named by President Obama as recipients of the Presidential Early Career Award for Scientists and Engineers, the highest honor bestowed by the United States government on science and engineering professionals in the early stages of their independent research careers. In addition, Professor Nolan was selected by the School of Science as the recipient of the 2016 Teaching Prize for Graduate Education, a reflection of her outstanding abilities as an educator. These prizes are awarded annually to School of Science faculty members who demonstrate excellence in teaching in their subjects.

Professor Bradley L. Pentelute, the Pfizer-Laubach Career Development Associate Professor of Chemistry, was named the recipient of the 2017 Bristol-Myers Squibb Unrestricted Grant in Synthetic Organic Chemistry. Launched in 1977, the Bristol-

Myers Squibb Freedom to Discover Grants and Awards Program embodies a vision of partnership between private industry and academic research to promote innovative scientific discovery.

In March 2017, a team led by Professor Gabriela Schlau-Cohen, the Cabot Career Development Professor of Chemistry, was selected by the International Human Frontier Science Program Organization as the winner of a Young Investigator Grant. Also, Professor Schlau-Cohen was named a 2016 recipient of the Beckman Young Investigator Award. This award provides research support to promising young faculty members in the early stages of their academic careers in the chemical and life sciences, with a particular aim of fostering the invention of methods, instruments, and materials that will open up new avenues of research in science.

Professor Richard Royce Schrock, the F.G. Keyes Professor of Chemistry, was named the recipient of the 2017–2018 James R. Killian, Jr. Faculty Achievement Award. Established in 1971 to honor Killian, MIT's 10th president, the award recognizes extraordinary professional achievements by an MIT faculty member.

In January 2017, Professor Matthew D. Shoulders, the Whitehead Career Development Professor, was selected to receive a National Science Foundation (NSF) CAREER Award for his proposal "Integrating Chemical Biology Methods and RNA Virus Models to Elucidate How the Metazoan Proteostasis Network Modulates Protein Evolutionary Landscapes." The CAREER program offers NSF's most prestigious awards in support of junior faculty who exemplify the role of teacher-scholars through integration of education and research within the context of the mission of their organizations.

In July 2017, Professor Susan Solomon, the Lee and Geraldine Martin Professor of Environmental Studies, was awarded the UK Royal Society's prestigious Bakerian Medal in honor of "her outstanding contributions in atmospheric science, in particular to the understanding of polar ozone depletion." The historic Bakerian Medal and Lecture was established in 1775. Also, Professor Solomon was awarded the 2017 National Academy of Sciences Arthur L. Day Prize and Lectureship. The Day Prize and Lectureship honors a scientist who is making lasting contributions to the study of the physics of the Earth and whose lectures will provide solid, timely, and useful additions to the knowledge and literature in the field.

In February 2017, Professor Yogesh Surendranath was named a 2017 Cottrell Scholar by the Research Corporation for Science Advancement. The Cottrell Scholar program champions the best early-career teacher-scholars in chemistry, physics, and astronomy by providing significant discretionary awards.

In May 2017, Professor Troy Van Voorhis and Professor Surendranath were awarded one of 10 early-stage energy research seed fund grants (each in the amount of $150,000) for their project "Computational Design and Synthesis of Graphene Based Fuel Forming Catalysts."

In December 2016, Professor Adam Willard was named the recipient of an NSF CAREER Award for his proposal "Characterizing Water's Response to Hydrophilic Surfaces." In addition, Professor Willard was named a 2017 Cottrell Scholar.

Development News

When the MIT.nano building is dedicated in 2018, two spaces in the new building will be named for major supporters of the Department of Chemistry. 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, will have the conference room adjacent to the chemistry undergraduate teaching labs named in their honor for their gift of $500,000. The director’s office in the chemistry undergraduate teaching labs will be named for the Fred J. Brotherton Foundation in honor of a gift of $100,000 facilitated by Dr. William B. Brotherton SB’72.

While graduate student support remains one of the principal fundraising priorities for the department, the other fundraising priority is renewal and replacement of critical instrumentation in the Department of Chemistry Instrumentation Facility (DCIF), a core facility (conveniently located at the center of the campus) for researchers not only in the department but across the campus and beyond. Of the seven nuclear magnetic resonance (NMR) instruments housed in the facility, the most recently acquired instrument was purchased in 1999. Selwyn Foundation trustees Lee and Judith Selwyn have kick-started our fundraising efforts for the DCIF with a lead gift of $100,000. Judy, as a member of the Department of Chemistry’s Visiting Committee, is acutely aware of these critical instrumentation needs. Other members of the committee have generously collectively contributed $60,500.

Planned Giving and Bequests

The department is gratified by the thoughtfulness and foresight of many of its alumni in establishing planned giving vehicles and bequests to ensure that the department remains strong going forward.

Graduate Student Support

The department is grateful to the following individuals for their continued major support of summer graduate students:

- Ping S. Chu PhD ’80
- Dr. Michael E. Strem
- Merece Johnson
- Daniel C. Harris SB ’68 and Sally L. Harris
- Kin Chun T. Luk PhD ’77 and Yuen-Kwan Luk
- Professor Jeffrey I. Steinfeld SB ’62
- T-Y Shen and Amy L. Shen
- Gregory C. Fu SB ’85
- Professor Stephen L. Buchwald and Dr. Susan Haber
- Dr. Jan Krouwer PhD ’73 and Ruby Krouwer

Other endowed funds that provide support for graduate students at varying levels are as follows:

- Lord Spectroscopy Fund
- Michael S. Feld Memorial Fellowship Fund
- Satoru Masamune Memorial Fund
- Richard R. Schrock Fellowship Fund
- Stephen J. Lippard Fellowship Fund
- Davison Prize Fund
- Davison Fellowship Fund
- Walter L. Hughes (1937) Memorial Fund (expendable)

Inaugural Waugh Lectureship

The department established the John S. Waugh Lectureship in Physical Chemistry through gifts from the Waugh family and friends. The inaugural lecture, "NMR Crystallography: 50 Years after WAHUHA," will be delivered by Dr. Lyndon Emsley (EPFL, Lausanne, Switzerland) on September 26, 2017.

Alumni and Friends Reception

Potential scientific solutions to global crises are welcomed and important in the face of environmental uncertainty. On April 25, the Department of Chemistry and the School of Science held an alumni and friends reception at which invited guests gathered in the Samberg Conference Center for an evening of food, drink, and talks by Professors Mircea Dincă and Gabriela Schlau-Cohen on their basic science research—research that can help mankind address global challenges involving food, water, and energy.

Named Lectures

The department welcomed the following named speakers during fall 2016 and spring 2017:

- Merck-Pfister Lecture in Organic Chemistry: Kyoko Nozaki, University of Tokyo
- MIT-Merck Lecture in Organic Chemistry: Donna Blackmond, Scripps, and Yves Ducharme, Merck
- Merck-Banyu Lecture in Organic Chemistry: Satoshi Maeda, Hokkaido University
- Boehringer-Ingelheim Lecture in Organic Chemistry: Paul Knochel, Ludwig-Maximilians-Universitat, and Daniel Fandrick, Boehringer-Ingelheim
- Davison Lecture in Inorganic Chemistry: Matthias Driess, Technische Universitat Berlin
- Georgia-Pacific Lecture in Organic Chemistry: Mark MacLachlan, University of British Columbia

- TY Shen Lectures in Biological Chemistry: Franz-Ulrich Hartl, Max Planck Institute of Biochemistry
- Merck-Pfister Lecture in Organic Chemistry: M.G. Finn, Georgia Institute of Technology
- Pfizer-MIT Lecture in Organic Chemistry: Gregory C. Fu, California Institute of Technology
- Buchi Lecture in Organic Chemistry: Eiichi Nakamura, University of Tokyo
- A.D. Little Lecture in Physical Chemistry: Arup Chakraborty, MIT

Serving the Institute

The Department of Chemistry provides key educational services to the Institute. During AY2017, the department taught 1,329 MIT undergraduate students in the areas of biochemistry and inorganic, organic, and physical chemistry. The department was also the home for 50 Undergraduate Research Opportunities Program (UROP) students, providing important mentoring relationships for students from a number of departments, including chemistry, biology, mathematics, physics, chemical engineering, biological engineering, and materials science.

Chemistry Majors

We continue to consistently attract a very talented group of undergraduates to Course 5, with a total of 40 majors across three years. This year, 21 students received SB degrees in chemistry. In exit surveys, we found that 38% of the members of the Class of 2017 are bound for graduate school and 10% plan to attend medical school; 33% will seek employment, and 19% were undecided as of commencement. Three of the students seeking employment are doing research abroad for a year.

At the end of the spring term, the new 5-7 major was announced and was popular immediately, with 20 students declaring chemistry and biology as their major. Of these students, 60% were from the Class of 2020, 20% from the Class of 2019, and 20% from the Class of 2018. These figures include four students within the department who changed their major from 5 to 5-7.

Undergraduate Research Opportunities Program

The Undergraduate Research Opportunities Program continues to be the capstone experience for our undergraduates. More than 80% of our majors work in a research group at least once during their degree program, conducting research alongside faculty, postdocs, and graduate students.

Chemistry Teaching Assistants

Our graduate student teaching assistants (TAs) are among the best at MIT. This year, students gave 77% of our TAs a 6.0 or higher rating on a 7.0 scale. Of the TAs in this percentile, 49% received a rating of 6.5 or higher.

Lisa Cunden received the 2016–2017 Department of Chemistry Award for Continued Excellence in Teaching.

Undergraduate Awards

- Freshman Chemistry Achievement Award (for outstanding academic achievement in chemistry): Alexander Alabugin, Hikari Iwasaki, and Priscilla Liow
- Outstanding Sophomore Achievement Award (for outstanding achievement in academics, research, and service to the Department of Chemistry): Min Woo Bae
- ACS Analytical Chemistry Award (for outstanding achievement by a junior in experimental chemistry): David Vaccaro
- Outstanding UROP Presentation Award (for outstanding undergraduate research and in recognition of the best presentation at the 2016 Chemistry UROP Symposium): Tomohiro Soejima
- Alpha Chi Sigma Award (for outstanding achievement in scholarship, research, and service to the Department of Chemistry): James Deng Aofei Liu
- Research Award (for outstanding contributions in the area of research): Jessica Gable, Nicholas Garcia, Jiwon Park, and Ian Perry
- Frederick D. Greene Teaching Award (for outstanding contributions in the area of teaching): Sebasthian Santiago and Justin Bader
- ACS Inorganic Chemistry Award (for excellence in inorganic chemistry): Tomohiro Soejima
- ACS Organic Chemistry Award (for excellence in organic chemistry): James Deng
- Merck Index Award (for outstanding scholarship): Tomohiro Soejima
- Service Award (for significant contributions in the area of service to the Department of Chemistry): Nicholas Garcia and Tomohiro Soejima
- Phi Beta Kappa 2017 inductees: Alexander Clifton, James Deng, Aofei Liu, and Tomohiro Soejima
- Teaching Assistant Awards: Kyan D'Angelo, Amr Dodin, Jesse Gordon, Andrew Licini, Katie McGeough, Lexie McIsaac, Andrew Navia, Carly Schissel, Alexander Shcherbakov, Scott Shepard, Shwetha Srinivasan, Erica Tsai, Cassie Zentner, Kristin Zuromski, Emily Zygiel

Doctoral and Master's Degree Recipients

September 2016

Name	Degree	Group
Khalid Al Kaabi	SM	Dincă group
Pedro Arrechea	PhD	Buchwald group
Laura Avena	SM	Cummins group
Jose Cordero Hernandez	PhD	Bawendi group
Igor Coropceanu	PhD	Bawendi group
Kurt Cox	PhD	Bawendi group
Kathleen Martin	SM	Dincă group
Anont Tanaset	SM	Van Humbeck group

February 2017

Name	Degree	Group
Anmol Gulati	SM	Nolan group
Whitney Hess	PhD	Bawendi group
Elizabeth Kelley	PhD	Jamison group
Jenny Liu	PhD	Johnson group
Toshiki Nakashige	PhD	Nolan group
Mackenzie Parker	PhD	Stubbe group
Mark Simon	PhD	Pentelute group
Yongbao Sun	PhD	Nelson group
Alexander Vinogradov	PhD	Pentelute group
Kolby White	PhD	Movassaghi group

June 2017

Name	Degree	Group
Thach Can	PhD	Griffin group
John Fennell	PhD	Swager group
David Grimes	PhD	Field group
Ken Kawamoto	PhD	Johnson group
Eric Keeler	PhD	Griffin group
Ioana Knopf	PhD	Cummins group
Markrete Krikorian	PhD	Swager group
Jian Lu	PhD	Nelson group
Sarah Luppino	PhD	Swager group
Thomas McTeague	PhD	Jamison group
Surin Mong	PhD	Pentelute group
Matthew Nava	PhD	Cummins group
Charles Ocampo	PhD	Jamison group
Satapanawat Sittihan	PhD	Jamison group
Prasahnt Sivarajah	PhD	Nelson group
Julia Stauber	PhD	Cummins group
Paul Stevenson	PhD	Tokmakoff group
Lei Sun	PhD	Dincă group
Amanda Wicker	SM	Jamison group
Elizabeth Wittenborn	SM	Drennan group
Chi Zhang	PhD	Pentelute group

Faculty Research Highlights

Stephen L. Buchwald

The Buchwald research group continues to develop novel methods for the formation of carbon-carbon and carbon-heteroatom bonds. The methods they develop are used to construct complex, biologically relevant compounds. Starting with simple precursors (alkenes), the use of copper-catalyzed methods allows for highly selective synthesis of enantiomerically enriched amines and aziridines and asymmetric synthesis of carbon-carbon bonds. Additionally, mechanistic studies led to the development of new precatalysts and ligands for palladium-catalyzed cross-coupling reactions. Also, continuous flow technology was used to rapidly generate and safely handle thermally unstable intermediates for the synthesis of fluoro- and trifluoromethyl-substituted compounds, which are ubiquitous structural components in many pharmaceuticals and agrochemicals. Furthermore, in collaboration with Professor Pentelute and his group, the Buchwald group developed new techniques for the functionalization of biomolecules.

Sylvia T. Ceyer

The Ceyer group continues to explore a fundamental dynamic principle applicable to the development of more efficient reactivity at the interfaces of covalent solids by investigating the non-equilibrium effects of multiple collisions in semiconductor etching. The group is also continuing to investigate a low-energy pathway for dissolution of hydrogen into the bulk of a nickel (Ni) alloy. This alloy is an excellent model for the Raney Ni catalyst, used commercially in all heterogeneous catalytic hydrogenation reactions.

Arup K. Chakraborty

The Chakraborty lab continued its efforts to understand the mechanistic bases of how a specific and systemic immune response to pathogens 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. Over the past year, Chakraborty, in collaboration with Professors Philip Sharp and Richard Young, launched a new project focused on understanding how genes critical for maintaining healthy cell states are regulated.

Christopher C. Cummins

The Cummins lab reported on fundamental reactivity studies of peroxide dianion that have implications for next-generation lithium-air battery technology and reveal why this technology is not compatible with carbon dioxide. A new family of cis-macrocyclic diphosphines was synthesized in only three steps from elemental phosphorus; the new ligands were tested and found to be effective in nickel-catalyzed coupling of ethylene with carbon dioxide. Simple main-group element compounds were studied through negative-ion photoelectron spectroscopy in an effort to understand the origins of the special stability of these unusual multiply bonded systems. Metaphosphate ligands were shown to stabilize terminal titanyl complexes and to have a ligand field strength similar to that of water.

Rick L. Danheiser

In AY2017, the Danheiser laboratory published a method for synthesizing highly substituted aromatic compounds using a “benzannulation” strategy in which the aromatic ring system is assembled from simple non-cyclic building blocks. This environmentally friendly chemical reaction generates no byproducts other than molecular nitrogen and is triggered by light through a continuous flow process that conveniently allows for large-scale work.

Mircea Dinca

The Dincă lab demonstrated a first example of a non-carbon-containing electrochemical double-layer supercapacitor and a new material with a record uptake of water from the atmosphere, providing important alternatives to electrical energy storage and fresh water production.

Catherine L. Drennan

A major finding in the Drennan lab in 2016–2017 was that more than 7,000 enzymes of the 100,000-member radical S-adenosylmethionine (SAM) enzyme superfamily require vitamin B_{12} for activity. These B_{12}-dependent radical SAM enzymes function in the biosynthetic pathways of compounds that include chlorophyll, the antibiotic fosfomycin, the herbicide bialaphos, and the antiviral compound oxetanocin-A. The Drennan laboratory determined the first crystal structure of a B12-dependent radical SAM enzyme.

John M. Essigmann

Liver cancer is invariably fatal if not detected early and has four causes: the food contaminant aflatoxin B1, alcohol abuse, and the hepatitis B and C viruses. The Essigmann laboratory used a new DNA sequencing technique that is over three orders of magnitude more sensitive than conventional sequencing to identify the mutagenic fingerprint of aflatoxin. The high sensitivity of the technique allowed the group to see the mutagenic signature of aflatoxin as early as 10 weeks after a single exposure to the liver toxin. They then used informatics tools to identify the aflatoxin fingerprint in the sequences of a subset of 314 human liver cancers that had been sequenced. The tool can next be applied to "liquid biopsies" to identify liver cancer at an early stage, when removal by surgery is still possible.

Robert W. Field

The unequal SO bond lengths in the C electronic excited state of SO2 and the very low vinylidene to acetylene isomerization barrier are caused by strong vibronic coupling interactions with a high-lying electronically excited state. The vinylidene isomerization barrier, viewed in the photoelectron spectrum, was made possible by the Field lab's observation of vibronically allowed bands and proven by photoelectron anisotropy.

Robert Guy Griffin

The Griffin group determined the structure of Aβ1-42 fibrils, the toxic species in Alzheimer's disease (AD), which affects more than 5.5 million people in the United States alone. This structure, which has been unknown since the first diagnosis of AD more than 100 years ago, was determined using a variety of new magic angle spinning NMR techniques developed by the Griffin group over the last decade. These "dipole recoupling" methods permitted the determination of more than 500 structural constraints and the first truly high-resolution structure of the Aβ1-42 dimer that occurs in fibrils. Research is proceeding on additional fibers associated with AD and with other amyloid-based diseases.

Mei Hong

In AY2017, the Hong group revealed how an influenza virus membrane protein, M2, conducts protons asymmetrically from the endosome to the virus interior. Using solid-state NMR spectroscopy, they observed the structural transformations of a proton-selective amino acid residue, histidine, when a tryptophan is mutated to phenylalanine. Also, they showed that this tryptophan in the wild-type protein prevents protons from the virus interior from protonating the histidine, thus accomplishing unidirectional proton conduction. In addition, the Hong group studied how the M2 protein binds cholesterol in the lipid membrane to carry out membrane scission, which allows new viruses to be released from the host cell. By measuring cholesterol-protein distances and bound cholesterol orientation in the membrane using solid-state NMR, they determined the binding site and binding stoichiometry of cholesterol to M2, which provided novel insight into the mechanism of virus budding. Finally, the group used two-dimensional ^{13}C solid-state NMR to investigate how pectins in rapidly growing plant cell walls interact with cellulose on a molecular level. They found that pectins are more dynamic and less strongly bound to cellulose microfibrils in these cell walls, which supports the emerging concept that pectins play an important role in wall loosening and wall mechanics.

Barbara Imperiali

The Imperiali group applies multidisciplinary approaches to gain insight into the intricate membrane-associated pathways that lead to biogenesis of carbohydrate-modified proteins and lipids, which play critical roles in human health and disease. This year, they made major progress in understanding the structure and mechanism of a new superfamily of enzymes that catalyze the initiating step in these pathways. With this knowledge, they are strategically positioned to develop chemical tools that can be used to identify processes to target in the study of infectious disease.

Timothy F. Jamison

In collaboration with William H. Green (Department of Chemical Engineering), the Jamison group demonstrated the use of continuous flow chemistry, computational analysis, and solvent-reduction strategies to minimize chemical waste production during the synthesis of two important pharmaceuticals. The Jamison group also developed rapid and modular continuous flow syntheses of agrochemicals and pharmaceuticals that feature a fluorinated heterocyclic core. In addition, the first practical use of sulfur hexafluoride as a fluorinating agent in organic synthesis was demonstrated using photoredox catalysis.

Jeremiah A. Johnson

The Johnson group, in collaboration with Professor Bradley D. Olsen, developed a new theory of elasticity that quantitatively describes how cyclic defects in polymer networks impact their elastic modulus. Also, they developed a new visible-light catalyzed polymerization reaction that enables controlled synthesis of a wide range of polymers.

Stephen J. Lippard

On October 11, 2016, BTP-114, a platinum anticancer drug based on the Lippard group's work, was injected into the first patient in a Phase I clinical trial. The monofunctional platinum anticancer agent phenanthriplatin was identified as a potent inhibitor of topoisomerase II, a key enzyme responsible for untangling DNA. Strategies to deliver phenanthriplatin selectively to tumor sites in the body were developed with collaborators at Case Western Reserve University. The role that DNA repair enzymes play in promoting cisplatin hypersensitivity in testicular cancer was explored. New sensors for imaging mobile zinc that can be targeted to programmable sites in biological samples were synthesized and studied in live cells. The first ratiometric copper(II)-based fluorescent sensors for direct detection of nitric oxide were produced and characterized.

Mohammad Movassaghi

The Movassaghi lab continues to focus on the development of new strategies and technologies for complex molecule synthesis. They recently reported the first total syntheses of the complex alkaloid (+)-haplocidine and its amide congener natural product (+)-haplocine after applying their electrophilic amide activation chemistry to secure the core structure. Additionally, they discovered that agelastatin alkaloids are potent modulators for cancer invasion and metastasis at non-cytotoxic doses, and they described a platform for the rapid synthesis of agelastatin derivatives. They continue to gain inspiration from nature in designing their chemical syntheses of these complex molecules, and the solutions they have uncovered offer unparalleled efficiency and a high level of stereochemical control in complex settings.

Keith A. Nelson

The Nelson group had several signature achievements over the past year. They recorded THz-frequency electron paramagnetic resonance (EPR) spectra of organometallic compounds in collaboration with Professor Dincă and his group, extending EPR measurements of electron spin states into the THz range with a simple methodology for the first time. They conducted the first measurements of photogenerated acoustic waves and submicron heat transport at extreme ultraviolet (EUV) wavelengths at a unique EUV free-electron laser facility in Trieste, Italy. Also, in collaboration with Professor Christopher Schuh (Department of Materials Science and Engineering), the Nelson group used intense laser pulses to initiate hypervelocity particle impact, observing in real time as metallic particles either stuck to or rebounded from metallic surfaces. Finally, they published the results of a comprehensive study of the liquid-glass transition in a viscoelastic fluid, using (in collaboration with a Danish research group) seven different experimental methods to probe mechanical and acoustic responses spanning 13 decades of frequencies, from millihertz to gigahertz.

Elizabeth M. Nolan

The Nolan lab discovered that the metal-chelating antimicrobial protein human calprotectin can sequester nickel ions and thereby inhibit the urease activity of *Staphylococcus aureus* and *Klebsiella pneumoniae*, two human pathogens that require nickel when colonizing the urinary tract. Their results suggest that, during the innate immune response against invading microbial pathogens, calprotectin may contribute to a nickel-withholding response at certain infection sites. In studies of human defensin peptides, the laboratory found that the small intestinal peptide HD6 can suppress the virulence traits of *Candida albicans*, an opportunistic fungal pathogen that typically lives in the human gut as a harmless commensal organism. HD6 prevents *C. albicans* from adhering to host epithelial cells and inhibits biofilm formation.

Bradley L. Pentelute

This past year, the Pentelute lab built a machine that enables the use of chemistry to prepare drug molecules in minutes at research scales. They believe this technology will aid in the development of personalized cancer vaccines.

Alexander T. Radosevich

The Radosevich lab reported on new roles for phosphorus-based compounds in catalytic transformations. The group discovered a catalytic hydroboration of imines in which B-H bond activation proceeded via bifunctional addition across one P-N linkage in a phosphorous triamide. In other work, they focused on catalytic syntheses of heterocycles (indazoles and benzimidazoles).

Gabriela S. Schlau-Cohen

This year the Schlau-Cohen lab learned that moss and algae protect themselves from too much sunlight by converting excess energy to heat. They also demonstrated that energy transfers more efficiently when excited states are delocalized over multiple molecules. In addition, the group found that the membrane holding photosynthetic proteins affects the time scales of energy transfer in light harvesting.

Richard R. Schrock

In AY2017, the Schrock lab discovered how to employ electron-poor olefins in olefin metathesis reactions. This discovery should dramatically expand the possible applications of olefin metathesis to synthesis of complex organic molecules. They also uncovered a molybdenum catalyst for reducing molecular nitrogen with protons and electrons, which may bring them closer to a practical synthesis of ammonia from protons and electrons that avoids the production of carbon dioxide on the large scale currently observed in the Haber-Bosch process.

Alex K. Shalek

Over the past year, the Shalek lab has broadly applied "Seq-Well," the group's ultra-high-throughput, low-cost, microwell-based single-cell RNA-Seq platform, to systematically examine how cellular composition and communication drive healthy and diseased tissue behaviors. Through local, national, and international collaborations (in England, Spain, Switzerland, Malawi, South Africa, and Thailand), they have profiled a wide array of human, non-human primate, and murine tissue isolates to define their cellular structures as well as deviations induced by different cancers (e.g., pancreatic, colon, and lung cancers and brain metastases), infections (e.g., *Mycobacterium tuberculosis* in lung tissue and cerebrospinal fluid), and inflammatory diseases (e.g., respiratory inflammation in nasal epithelia and ulcerative colitis in gut mucosa). While each project alone is affording unprecedented insights into the relevant disease etiologies, taken together they are beginning to reveal common cellular motifs that inform healthy tissue equilibria and immune behaviors and novel therapeutic and prophylactic paradigms. In parallel, the group is actively developing new technologies to facilitate deeper, more mechanistic inquiries into the factors that influence the social structure and fitness of cellular ensembles.

Matthew D. Shoulders

The Shoulders lab designed a methodology to control the levels of any endogenous protein in any cell model system of interest using an otherwise biologically inert small molecule. They also discovered that human host mechanisms that normally assist the folding of autonomous proteins are often hijacked by RNA viruses to assist their evolution, thereby likely contributing to rapid antiviral drug resistance onset. Other highlights included significant progress toward the development of the first widely adaptable platform for directed evolution in human cells.

Yogesh Surendranath

The Surendranath group aims to use electricity to rearrange chemical bonds by manipulating interfacial reactivity at the molecular level. Over the last year, they have developed a new class of porous silver catalysts for the selective and tunable conversion of carbon dioxide to carbon monoxide. In addition, they have characterized the population of the key carbon monoxide intermediate bound to copper surfaces during electrochemical fuel formation and developed a membrane-free formate fuel cell that operates under benign neutral pH conditions.

Timothy M. Swager

The Swager group has developed a novel method for the detection of pathogenic bacteria with a simple assay that can be read by a smartphone. This method has the potential for real-time detection of pathogens in food during the production cycle and could prevent outbreaks of food-induced illness. Another emerging area of focus in the group is the development of magneto-optical materials that could be used to create sensors allowing for the detection of low magnetic fields. These sensors can be employed for tracking of submarines or tracking of self-driving cars to detect the approach of other cars without a line-of-sight optical signal.

Jeffrey Van Humbeck

Almost all organic chemicals have numerous carbon-hydrogen (C-H) bonds. The Van Humbeck laboratory works toward developing new tools to convert specific C-H bond into new bonds commonly found in pharmaceuticals. Over the last year, they have expanded upon their initial 2016 discovery and can now selectively convert certain C-H bonds into carbon-oxygen, carbon-nitrogen, and carbon-fluorine bonds.

Troy Van Voorhis

In the past year, the Van Voorhis group has continued its focus on fragment-based methods that could accelerate electronic structure calculations for large systems by orders of magnitude. The group has also begun a significant effort to understand the physical and electronic structure of quantum dots and semiconductor surfaces, with an emphasis on the influence of surface states on processes such as energy and electron transfer.

Adam Willard

The Willard group published a paper illustrating how metal-water interactions influence separation of charged molecules near an electrode surface. Also, in collaboration with other researchers at MIT, the group published papers focused on predicting the microscopic organization of molecules within a self-assembled polymer gel, describing how surface-bound molecules influence the shape deformations of semiconductor nanocrystals, and understanding how disorder affects transient photoluminescence in quantum dot solids.

Bin Zhang

The Zhang group has developed a theoretical model to enable de novo prediction of three-dimensional genome structures using DNA sequences and histone modifications. This model will help reveal the role of genome organization in gene regulation and cell differentiation. The group has also characterized the unfolding pathway of the nucleosome with atomistic detail and provided a mechanistic understanding of various key observations from single-molecule pulling experiments.

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