Department of Chemistry

In academic year 2018, the Department of Chemistry had 31.5 full-time faculty (including two dual faculty appointments, one with the Department of Biological Engineering and one with the Institute for Medical Engineering and Science [IMES]): seven assistant professors, two associate professors without tenure, four associate professors with tenure, and 18.5 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 Stephen Lippard retired from teaching in the summer of 2017, and Professor Jeff Van Humbeck 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 275 graduate students, 118 postdoctoral researchers, and 53 undergraduate chemistry majors.

Professors Mircea Dincă and Bradley L. Pentelute were awarded tenure effective July 1, 2017. The department welcomed Professors Laura L. Kiessling and Ronald T. Raines, both from the University of Wisconsin, in July 2017.

In AY2018, the School of Science named Robert Guy Griffin the Arthur Amos Noyes Professor of Chemistry and Susan Solomon the Lee and Geraldine Martin Professor in Environmental Studies. The School also appointed Gabriela Schlau-Cohen to the Cabot Career Development Professorship and Alex K. Shalek to the Pfizer-Laubach Professorship.

Faculty Awards and Honors

Arup Chakraborty, the Robert T. Haslam Professor of Chemical Engineering and founding director of IMES, was named a 2018 Guggenheim Fellow by the John Simon Guggenheim Memorial Foundation. Also, Professor Chakraborty was elected to the National Academy of Medicine in recognition of his distinguished contributions to medicine and health.

Professor Dincă was named one of 31 US national finalists for the 2018 Blavatnik Award. He was selected as a finalist in the life sciences category for his boundary-pushing work in the area of metal-organic frameworks. In addition, Professor Dincă received the 2018 American Chemical Society (ACS) Award in Pure Chemistry. This award recognizes and encourages fundamental research in pure chemistry carried out by young men and women in North America.

Professor Robert Guy Griffin was awarded the 2017 Richard R. Ernst Prize in Magnetic Resonance. The prize recognizes ground-breaking applications of new or previously known techniques in all areas of magnetic resonance, published in the last three years.

Timothy F. Jamison—head of the Chemistry Department and Robert R. Taylor Professor of Chemistry—and graduate student Michelle MacLeod (PhD '18) were presented a 2018 Change Maker Award for the department's efforts to enhance education and training for faculty, students, and staff. Jamison and MacLeod were selected and highlighted as a model for other MIT departments to follow.

Professor Jeremiah A. Johnson was named the co-recipient of the 2018 Biomacromolecules/Macromolecules Young Investigator Award. He received the award for his contributions in developing polymer synthesis methods that provide macromolecules with novel functions in polymer physics. In April 2018, Professor Johnson was named to the Stand Up to Cancer (SU2C) Multiple Myeloma Dream Team. This dream team is the 23rd announced by SU2C since its inception in 2008 and the first devoted entirely to a hematologic malignancy. In December 2017, the School of Science awarded Professor Johnson the prize for undergraduate education for his role in 5.43 Advanced Organic Chemistry. In addition, Johnson and his former graduate student Aleksandr V. Zhukovitskiy (PhD '16) were named winners of the ACS Nobel Laureate Signature Award for Graduate Education in Chemistry. This award recognizes outstanding graduate students and their preceptors in the field of chemistry.

In June 2018 Stephen J. Lippard, the Arthur Amos Noyes Emeritus Professor of Chemistry, was awarded an honorary doctorate from the Hebrew University of Jerusalem.

In September 2017, Professor Laura L. Kiessling was awarded the Tetrahedron Prize for Creativity in Organic Chemistry for her outstanding contributions to organic chemistry. She was the first woman to be chosen for this illustrious award and joined an impressive list of past winners that includes several Nobel Laureates.

Keith A. Nelson, the Haslam and Dewey Professor of Chemistry, was presented the 2018 Frank Isakson Prize for Optical Effects in Solids by the American Physical Society. Nelson was selected for his pioneering contributions to the development and application of ultra-fast optical spectroscopy to condensed matter systems and for providing insight into lattice dynamics, structural phase transitions, and non-equilibrium control of solids.

Bradley L. Pentelute, the Pfizer-Laubach Career Development Associate Professor of Chemistry, was named one of 31 US national finalists for the 2018 Blavatnik Award. He was selected as a finalist in the life sciences category for his work on synthesizing new biomolecules for therapeutic compounds.

Gabriela Schlau-Cohen, the Cabot Career Development Professor, was awarded a 2018 Sloan Research Fellowship. Sloan Research Fellowships are awarded each year to early-career scientists in recognition of distinguished performance and a unique potential to make substantial contributions to their field.

Alex K. Shalek, the Pfizer-Laubach Career Development Assistant Professor, was named a member of the 2018 class of Pew-Stewart Scholars for Cancer Research. The five independent early-career investigators who make up the class are revolutionizing cancer research and working toward a cure for the disease. Shalek received a four-year grant to advance his efforts. In addition, Professor Shalek was awarded a 2018 Sloan Research Fellowship.

Matthew D. Shoulders, the Whitehead Career Development Professor, was awarded a research scholar grant from the American Cancer Society in support of his project, New Connections: Stress, Proteostasis, Sugars, and Cancer. The grant was made possible through the efforts of the Ellison Foundation, whose pioneering support for cancer care and research includes much-needed capital support for cancer facility investments; the

foundation will provide funding of roughly $800,000 over the next four years. Also, in June 2018, a research proposal submitted by Professor Shoulders was selected for funding by the G. Harold and Leila Y. Mathers Foundation. The foundation's grant will enable a key project in his lab for the next three years. In addition, Professor Shoulders was one of 13 young faculty nationwide to be named a winner of the Camille Dreyfus Teacher-Scholar Award. The Camille Dreyfus Teacher-Scholar Awards Program supports the research and teaching careers of talented young faculty in the chemical sciences. In April 2018, Professor Shoulders received a Committed to Caring (C2C) Award from the Office of Graduate Education. By recognizing the human element of graduate education, the C2C Award aims to encourage good advising and mentorship across MIT's campus.

Professor Susan Solomon was awarded the 2018 Crafoord Prize for fundamental contributions to understanding the role of atmospheric trace gases in Earth's climate system. The prize is awarded by the Royal Swedish Academy of Sciences and the Crafoord Foundation. Awards are presented in one of four disciplines each year: mathematics and astronomy, geosciences, biosciences, or polyarthritis. In July 2017, Professor Solomon 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.

In June 2018 Timothy Manning Swager, the John D. MacArthur Professor of Chemistry, was awarded one of nine seed fund grants of $150,000 from the MIT Energy Initiative. The Seed Fund Program is an annual competition that supports early-stage innovative research across the energy spectrum. The research of Swager's team focuses on new approaches to generating polymer membranes with three-dimensional porosity. Professor Swager was also named a 2018 Vannevar Bush Faculty Fellow by the US Department of Defense (DoD). The Vannevar Bush Faculty Fellowship program, sponsored by the Office of the Under Secretary of Defense for Research and Engineering and administered by the Office of Naval Research, seeks outstanding researchers to conduct transformative studies in areas of interest to the DoD. In addition, Swager received a Professor Amar G. Bose Research Grant in December 2017; this grant supports MIT faculty with the potential to develop innovative and potentially paradigm-shifting research ideas. Swager, along with John Hart (Department of Mechanical Engineering) and Dina Katabi (Computer Science and Artificial Intelligence Laboratory), was awarded the grant for his development of a high-tech version of the bar codes used to identify everyday retail products.

In October 2017 JoAnne Stubbe, the Novartis Professor of Chemistry (emeritus), was named the recipient of the Pearl Meister Greengard Prize by The Rockefeller University.

Development

In 2017, Department Head Jamison made raising funds for instrumentation renewal and replacement in the Department of Chemistry Instrumentation Facility a high priority. In recognition of the importance of providing an up-to-date facility that supports research groups in the department and throughout MIT, the dean of science and the Institute committed to matching all gifts and pledges up to $1 million until June 30, 2018.

Professor Jamison was delighted to announce on June 30 that the $1 million fundraising goal was reached after Judith E. Selwyn PhD ’71 and her husband, Lee L. Selwyn PhD ’69, contacted the department with an offer to pledge a further $30,000, bringing the total to the $1 million needed to fully reach the matching agreement. The Selwyns had kick-started the mini-campaign in May 2017 with a lead gift of $100,000.

“We were the first to contribute to the match, and we were also happy to be the last to round it out to $1 million,” said the Selwyns. Judith is a member of the Department of Chemistry Visiting Committee and, as such, was acutely aware of the critical need to fully update the facility. Other members of the Visiting Committee collectively contributed $60,000, and the Department of Chemistry matched those contributions with $60,000. The remaining funds to bring the fundraiser to its successful conclusion were derived from other generous alumni and friends of the department.

Graduate Student Support

Graduate student support remains a fundraising priority. The department is grateful to the following individuals for their continued support of graduate students:

- Ping S. Chu PhD ’80
- Michael E. Strem
- Merece Johnson
- Daniel C. Harris SB ’68 and Sally L. Harris
- Kin Chun T. Luk PhD ’77 and Yuen-Kwan Luk
- Jeffrey I. Steinfeld SB ’62
- T-Y Shen and Amy L. Shen
- Gregory C. Fu SB ’85
- Professor Stephen L. Buchwald and Susan G. Haber
- Jan Krouwer PhD ’73 and Ruby Krouwer
- Charles Wade PhD ’65 and Kim Wade
- Kenneth M. Gordon ’76

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

- George H. Büchi Fund
- Richard C. Lord Spectroscopy Fund
- Michael S. Feld Memorial Fellowship Fund
- Satoru Masamune Memorial Fund
- Richard R. Schrock Fellowship Fund

- Stephen J. Lippard (1965) Fund
- Davison Prize Fund
- Davison Fellowship Fund
- Walter L. Hughes (1937) Memorial Fund

When the MIT.nano building is dedicated in October 2018, two spaces in the new building will be named for major supporters of the department. Judith E. Selwyn and Lee L. Selwyn 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 in honor of the Fred J. Brotherton Foundation for its gift of $100,000, facilitated by William B. Brotherton SB '72.

Alumni and Friends Reception

Professors Elizabeth M. Nolan and Jeremiah A. Johnson shared their efforts to address some of the greatest challenges currently faced by the chemical sciences field at an alumni and friends reception hosted by the Department of Chemistry and the School of Science on May 16, 2018.

Nolan, whose research addresses the chemistry and biology of human innate immunity and microbial pathogenesis, spoke about her lab's use of biological chemistry, inorganic chemistry, and microbiology toolkits to decipher the interplay between human host-defense molecules and microbes and the evaluation of new strategies for treating and preventing microbial infections.

Johnson described his group's efforts to develop a drug-agnostic materials platform that can enable rapid improvement of therapeutic indexes for drugs with known targets and established efficacy but poor safety profiles.

Named Lectures

The department welcomed the following named speakers during fall 2017 and spring 2018:

- J.S. Waugh Lecture in Physical Chemistry: Lyndon Emsley, EPFL (École polytechnique fédérale de Lausanne)
- Merck-Banyu Lecture in Organic Chemistry: Tomoki Ogoshi, Kanazawa University
- MIT-Merck Lecture in Organic Chemistry: Anna K. Mapp, University of Michigan, and Artis Klapars, Merck
- Davison Lecture in Inorganic Chemistry: Ib Chorkendorff, Technical University of Denmark
- Merck-Pfister Lecture in Organic Chemistry: Shigehiro Yamaguchi, Nagoya University
- Bristol-Myers Squibb Lecture in Organic Chemistry: Jennifer A. Prescher, University of California, Irvine, and Ke Chen, Bristol-Myers Squibb

- A.D. Little Lecture in Physical Chemistry: Taekjip Ha, Johns Hopkins University
- TY Shen Lectures in Chemical Biology: J. Martin Bollinger, Pennsylvania State University
- Novartis Lecture in Organic Chemistry: James S. Nowick, University of California, Irvine, and Aimee Usera, Novartis
- MIT-Pfizer Lecture in Organic Chemistry: Scott E. Denmark, University of Illinois
- Büchi Lecture in Organic Chemistry: Alois Fürstner, Max-Planck-Institut
- Chemistry in Industry Seminar: Timothy J. Oyer, Wolf Greenfield
- Chemistry in Industry Seminar: Alexandra Gould, Takeda International

Serving the Institute

The Department of Chemistry provides key educational services to the Institute. During AY2018, the department taught 1,249 MIT undergraduate students in the areas of biochemistry and inorganic, organic, and physical chemistry. The department was also the home for 55 Undergraduate Research Opportunities Program (UROP) students, providing important mentoring relationships for students from a number of departments, including chemistry, 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 and Course 5-7, with a total of 53 majors across three years (30 in Course 5 and 23 in Course 5-7). This year, 11 students received SB degrees in chemistry (six in Course 5 and five in Course 5-7). In exit surveys, we found that 27% of the members of the Class of 2018 will be attending graduate school and 45% will seek employment. Of the students seeking employment, 40% plan to attend graduate school in the near future and 40% plan to attend medical school after a year of employment. The post-MIT plans of the remaining students are unknown.

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 some of the best at MIT. This year, students gave 76% of our TAs a 6.0 or higher rating on a 7.0 scale. Of the TAs in this percentile, 58% received a rating of 6.5 or higher.

Undergraduate Awards

Awarded at the Undergraduate Recognition Banquet on May 15, 2018:

- Freshman Chemistry Achievement Award (for outstanding academic achievement in chemistry): Owen Broderick, Alexandra Dima, Ruiwen (Doris) Fu, Benjamin Nguyen, and Harrison Wang
- Outstanding Sophomore Achievement Award (for outstanding achievement in academics, research, and service to the Department of Chemistry): Hikari Iwasaki, Corin Wagen, and Sherry Zhou
- ACS Analytical Chemistry Award (for outstanding achievement by a junior in experimental chemistry): Min Woo Bae
- Outstanding UROP Presentation Award (for outstanding undergraduate research and in recognition of the best presentation at the 2018 Chemistry UROP Symposium): Corin Wagen
- Alpha Chi Sigma Award (for outstanding achievement in scholarship, research, and service to the Department of Chemistry): Coral Bays-Muchmore
- Research Award (for outstanding contributions in the area of research): Samuel Gordon and Mercedes Ondik
- Royal Society of Chemistry Certificate of Excellence (for outstanding scholarship): Camilo Espinosa, Alexander Turner, and David Vaccaro
- Service Award (for significant contributions in the area of service to the Department of Chemistry): Samuel Gordon
- Phi Beta Kappa 2018 inductees: Alexander Turner and David Vaccaro
- Teaching Assistant Awards: Grace Ahlqvist, Chris Breen, Aurelio Dregni, Steph Hart, Onyu Jung, Nathan Klein, Lennon Luo, Sarah Jane Mear, Chloe Morgan, Aditya Nandy, Jeff Rosenberg, Azin Saebi, Yuchen Sun, Eric Sung, Madeleine Sutherland, Katherine Taylor, Henry Tran, and Francesca Vaccaro

Doctoral and Master's Degree Recipients

September 2017

Name	Degree	Group
Jun Jiang	PhD	Field group
Pornchai Kaewsapsak	PhD	Ting group
Shu-Yu Liao	PhD	Hong group
Yi-Chun Li	PhD	Radosevich group
Sarah Park	PhD	Dincă group
Jonathan Williams	PhD	Hong group
Wanqin Xie	PhD	Welsch group

February 2018

Name	Degree	Group
Chern Chaung	PhD	Cao group
Yue Chen	PhD	Bawendi group
Peng Dai	PhD	Penteleute group
Andrew DiChiara	PhD	Shoulders group
Tyler Harrison	SM	Radosevich group
Alexander Kohn	PhD	Van Voorhis group
Wankyu Lee	PhD	Stubbe group
Petra Lindovska	PhD	Movassaghi group
Jingjing Ling	PhD	Ploegh group
Michelle MacLeod	PhD	Johnson group
Andrew Maher	PhD	Nocera group
Qing Zhe Ni	PhD	Griffin group

June 2018

Name	Degree	Group
Alyssa Antropow	PhD	Movassaghi group
Jessica Carr	PhD	Bawendi group
Sterling Chu	PhD	Surendranath group
Wen Chyan	PhD	Raines group
Leora Dresselhaus-Cooper	PhD	Nelson group
Ethan Evans	PhD	Pentelute group
Colin Fadzen	PhD	Pentelute group
Daniel Franke	PhD	Bawendi group
Emily Garnett	PhD	Raines group
Yicong Ge	SM	Dincă group
Aaron Goodman	PhD	Tisdale group
Tsehai Grell	PhD	Drennan group
Laurel Heckman	PhD	Jamison group
Byungsu Kwon	PhD	Hong group
Zeyang Li	PhD	Ploegh group
Qing Liu	PhD	Ceyer group
Eric Metzger	PhD	Dincă group
Alexander Mijalis	PhD	Pentelute group
Christopher Moore	PhD	Shoulders group
Brandon Nelson	PhD	Movassaghi group
Ricardo Pablo Pedro	PhD	Van Voorhis group
Thomas Parsons	SM	Zhang group
Angela Phillips	PhD	Shoulders group
Sucheol Shin	PhD	Willard group
Jules Stephan	PhD	Nolan group
Justin Wolfe	PhD	Nolan group
Anna Wuttig	PhD	Surendranath group
Jeffrey Yang	PhD	Buchwald group
Yuxuan Ye	PhD	Buchwald group
Youngmin Yoon	PhD	Surendranath group
Qifan Zhang	PhD	Swager group
Yunfei Zhang	PhD	Hatton group
Tianyu Zhu	PhD	Van Voorhis group

Faculty Research Highlights

Stephen L. Buchwald

The Buchwald research group focuses on the development of new reactions and methodologies for the formation of carbon-carbon and carbon-heteroatom bonds. The invention of new methods allows for highly efficient and selective construction of structural components prevalent in pharmaceuticals, materials, agrochemicals, and natural products. During the past year, the group developed new copper-hydride catalyzed techniques for the asymmetric synthesis of *N*-arylamines, amides, nitriles, and β-chiral aldehydes, and reported on a robust, large-scale protocol for copper-catalyzed hydroamination of alkenes. Mechanistic studies have enabled the design of new ligands and milder reaction conditions in palladium-catalyzed cross-coupling reactions. Additionally, in collaboration with Professor Pentelute's group, Buchwald and his team have developed new techniques for the functionalization of complex biomolecules.

Sylvia T. Ceyer

The Ceyer group continues to probe a fundamental dynamical 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. In addition, they are exploring the role of spin in semiconductor oxidation reactions and studying the acceleration of growth of a single layer of graphene on nickel (Ni).

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 an important facet as well. Chakraborty, in collaboration with Professors Philip Sharp and Richard Young, also launched a new project focused on understanding how genes critical for maintaining healthy cell states are regulated. Chakraborty is working on two books on immunology, one for an audience of physical scientists who want to enter (or have entered) the field and one for a general audience. Chakraborty co-chaired MIT's committee on Digital Health and continues to serve as a member of the US Defense Science Board, as well as a Senior Editor of *eLife*.

Christopher C. Cummins

The Cummins lab reported mechanistic studies on the generation of reactive intermediates known as phosphinidenes, the phosphorus analogs of carbenes, and their application to the synthesis of organophosphorus compounds. Also reported were new anthracene-eliminating reagents designed for carbon atom transfer, sulfur monoxide transfer, and methylene transfer. Finally, the lab described a potentially disruptive means of synthesizing phosphorus compounds starting from phosphoric acid, rather than from white phosphorus, as part of the Université Mohammed VI Polytechnique-MIT Research Program (UMRP) aimed at sustainable development in Africa.

Rick L. Danheiser

In AY2018, the Danheiser lab developed a new strategy for the chemical synthesis of the pyridine class of organic compounds. This method provides efficient access to compounds that have applications in medicine and biology as well as applications as agricultural chemicals.

Mircea Dinca

The Dincă lab has produced materials that hold a record for adsorption of water vapor from the atmosphere. These materials could be used for the production of fresh water in dry climates, such as the Sahara and the Middle East, addressing fresh water scarcity, one of the near future's most challenging problems.

Catherine L. Drennan

In AY2018 the Drennan lab, in collaboration with the Wilfred van der Donk laboratory at the University of Illinois, employed crystallography and molecular biology to determine sequence markers for the microbial synthase responsible for producing methylphosphonate (MPn), the natural product proposed to be the source of methane from the upper ocean. They found that MPn synthases are widely distributed among marine microbes, consistent with MPn production being extensive in the upper ocean and supporting the proposal that MPn is the source of oceanic methane release.

Robert W. Field

The Field group's goal is to prepare the NO^+ ion in a single vibration-rotation state: ($v^+ = 0, N^+ = 0$). They accomplish this through "vibrational auto-ionization" of a high orbital angular momentum ($\ell = 4$) Rydberg state of NO. The group has populated selected energy levels of NO(ng) complexes via three-laser triple resonance and measured the energies and decay rates of the $2\ell + 1 = 9$ fine structure components of each rotational level. The NO(ng) energy level patterns determine the dipole moment and polarizability of NO^+, and the decay rate pattern indicates whether the $\ell = 4$ Rydberg electron departs without exerting a torque on the NO^+ ion core. NO's evil tricks have frustrated all previous experimental attempts to exploit high-ℓ Rydberg states as a route to electronic characterization and rotation-selective population of NO^+. The Field group has vanquished NO!

Robert Guy Griffin

The Griffin group is performing structural experiments on amyloid fibrils related to Alzheimer's disease. They are also studying the transport of molecules across cell membranes and constructing a high-frequency pulsed dynamic nuclear polarization spectrometer.

Mei Hong

In AY2018, the Hong group made major strides in four scientific areas. They determined the membrane-bound structure of an antibody-targeted region of the HIV viral fusion protein, gp41. They showed that the antibody-targeted segment lies on the membrane surface, while the transmembrane segment spans the lipid bilayer and the protein

self-associates into trimers in the lipid membrane. This study is a first in that all prior structural investigations used short peptide fragments of this domain of gp41, and few studies were carried out in native virus-mimetic lipid bilayers. The group's results resolve many conflicting reports in the literature and set the stage for future development of anti-HIV vaccines. In addition, they discovered a millisecond-timescale conformational motion of the influenza M2 protein. The cooperative motion of the four-helix bundle between a low-pH conformer and a high-pH conformer provided the long-missing link of the rate-limiting step in proton transport by this influenza ion channel. The Hong group also carried out structure determinations of two important plant cell wall biopolymers, cellulose and sporopollenin. They elucidated the conformation of the most reactive moiety of cellulose, the hydroxymethyl group, using a ^{13}C-detected ^{1}H-^{1}H distance nuclear magnetic resonance (NMR) technique. The results show that the disordered β-(1,4) glucan chains on the cellulose microfibril surface adopt a different hydroxymethyl conformation from that of the interior crystalline chains. Using quantitative NMR and spectral editing methods, they determined, for the first time, the chemical makeup of sporopollenin, the inert biopolymer that is responsible for the survival of plant spores and pollen grains and the migration of early plants onto land. Finally, they developed two ^{19}F solid-state NMR approaches to measure internuclear distances of 1–2 nm. These distance techniques, designed for high magnetic field and fast magic-angle-spinning conditions, overcome the bottleneck of obtaining long-range distance constraints for high-resolution structure determination using solid-state NMR.

Barbara Imperiali

The Imperiali group applies multidisciplinary approaches to gain insight into the intricate membrane-associated pathways that lead to complex sugar-based polymers. These structures are displayed on the surface of cells and play critical roles in interactions among bacteria and between human cells and pathogenic and symbiotic bacteria. A major focus of the group has been on phosphoglycosyl transferases, which are key enzymes that initiate sugar polymer biosynthesis. They have discovered an entirely new superfamily of enzymes that are unique to bacteria and have defined the structure and mechanism of a representative member of the superfamily. They are now poised to understand the roles of these enzymes in human health and disease and to develop effective chemical probes to both monitor and inhibit their activities with the goal of defining novel targets in the study and treatment of infectious disease.

Timothy F. Jamison

In collaboration with Klavs F. Jensen and Allan Myerson (both of the Department of Chemical Engineering), the Jamison group developed a new-generation compact, reconfigurable continuous flow system that is capable of end-to-end pharmaceutical manufacturing. Potential applications include disaster relief and neglected diseases. The Jamison group also reported air-stable nickel complexes that are activated under mild conditions for homogeneous nickel catalysis and an efficient method for the synthesis of highly substituted 2-arylindoles, an important class of molecules found in natural products, therapeutics, and drug candidates.

Jeremiah A. Johnson

The Johnson group has developed a new type of polymeric material that can reversibly switch its topology in response to different wavelengths of light. They have also demonstrated the synthesis of block copolymers with precise length and stereochemistry. Using these polymers, they showed that stereochemistry alone can dictate the bulk morphology of uniform block copolymers. Finally, they introduced a scalable synthesis of star-shaped polymers that serve as angiotensin receptor blocker prodrugs. These polymers represent promising therapies for fibrotic disease.

Laura L. Kiessling

Watching enzymes in action as bacteria that build their cell walls can lead to new strategies to identify and treat them. The Kiessling group designed and synthesized a new probe, termed QTF (quencher-trehalose-fluorophore), that can be used to follow the assembly of the cell wall of mycobacteria, such as the bacteria that cause tuberculosis. QTF provides an understanding of the unique enzymes needed to build the mycobacterial cell wall, and thus it is the first bacterial imaging probe that can be used to follow cell division and growth. Because the cell wall of mycobacteria is different than that of other bacteria, this new probe also has the properties needed for a diagnostic agent and to uncover new drugs to treat diseases such as tuberculosis.

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 enantioselective total syntheses of the complex alkaloid (–)-deoxoapodine through application of electrophilic amide activation chemistry to secure the core structure. Additionally, using their diazene-directed fragment assembly, they developed the first completely stereoselective strategy for unions of whole cyclotryptamine substructures toward a synthesis of complex oligocyclotryptamine alkaloids. The group continues to gain inspiration from nature in designing their chemical syntheses of these complex molecules, and the solutions they have developed offer unparalleled efficiency and a high level of stereochemical control in complex settings.

Keith A. Nelson

The Nelson group had a particularly interesting year in the optical study and control of collective phenomena. They used terahertz-frequency light to induce electronic and structural phase transitions in novel materials (the single-molecular-layer transition metal dichalcogenides WSe_2 and MoS_2) and in a classical crystal, strontium titanate ($SrTiO_3$); their light field simply moved the ions into their positions in a new crystalline phase. In separate work, the group demonstrated wavelike heat transport at temperatures up to 150 K (about 10 times higher than ever observed previously), opening the door to possible practical applications at room temperature or higher. Finally, their studies of shock and particle impact showed unique results. The group was able to directly visualize shock-induced lattice deformation along particular crystallographic planes. Collaborating with a colleague from the Department of Materials Science and Engineering, they monitored individual metallic microparticle impacts that directly revealed the mechanism for particle adhesion to metallic targets in cold spray, an additive manufacturing method for which fundamental understanding had been elusive.

Elizabeth M. Nolan

The Nolan lab detected oxidized species of the metal-chelating antimicrobial protein calprotectin harboring methionine sulfoxide post-translational modification in samples of human mucus and pus. Further biophysical and biochemical evaluation of the protein uncovered oxidation of methionine 81 of the S100A9 subunit affects its quaternary structure and thereby accelerates its degradation by host serine proteases. Their work provides a new branch to the working model for calprotectin at infection sites, suggesting that post-translational oxidation of the protein by neutrophil-derived reactive oxygen species modulates its lifetime at extracellular sites. In studies of siderophore-antibiotic conjugates, the laboratory achieved proof-of-concept that the siderophore enterobactin can be used for the delivery of an antibiotic to the cytoplasm of *Escherichia coli*. This work included the discovery that a pathogen-associated esterase can be leveraged to activate an enterobactin-ciprofloxacin conjugate, providing antibacterial activity against only *E. coli* that express an enterobactin receptor in the outer membrane as well as the cytoplasmic enterobactin esterase IroD.

Bradley L. Pentelute

Over the past year, the Pentelute lab used machine learning to predict novel peptide sequences that deliver large oligonucleotides into cells. They believe this technology will aid in the development of personalized cancer vaccines and agents for the treatment of muscular dystrophy.

Alexander T. Radosevich

The Radosevich group has advanced the chemistry of low-symmetry phosphorus-based compounds in bond activation and catalytic transformations. Specifically, they developed a catalytic method for the synthesis of indoles and carbazoles involving phosphine/phosphine oxide redox cycling in a small ring phosphacyclic compound. Also, they reported the synthesis and reactivity of a chelating ligand containing a nontrigonal phosphorous triamide center that, upon metalation with a ruthenium hydride complex, yielded a chelated ruthenahydridophosphorane via net insertion into the Ru-H bond.

Ronald T. Raines

In AY2018, the Raines group developed a method to “cloak” the negative charges on proteins. Their cloaked proteins pass directly through the plasma membranes of mammalian cells. Inside, endogenous enzymes remove the cloak. Thus, their method provides a traceless way to deliver a protein to the cytosol and even the cellular nucleus.

Gabriela S. Schlau-Cohen

This year the Schlau-Cohen group demonstrated that the presence of one of the electronic excited states of carotenoids is controlled by the protein in photosynthesis. In addition, they constructed a biochemical platform to look at the protein epidermal growth factor receptor, which is the target for cancer drugs. The group also discovered that pressure from the biological membrane controls the pathways of energy flow in photosynthetic bacteria.

Richard R. Schrock

The Schrock lab discovered a new type of molybdenum catalyst for olefin metathesis reactions. This discovery is of fundamental interest and should dramatically expand the possible applications of olefin metathesis to the synthesis of complex organic molecules.

Alex K. Shalek

This year the Shalek lab (in collaboration with clinicians at Brigham and Women's Hospital) leveraged Seq-Well—the group's portable, low-cost, and nanowell-based platform for RNA sequencing of single cells at high throughput designed to be compatible with low-input, clinical biopsies—to systematically examine the cellular basis of the barrier tissue dysfunction that informs chronic allergic inflammation. Profiling minute primary human nasal surgical samples and scrapings spanning the disease spectrum—from mild inflammation (rhinitis) to severe polyposis—they reported the first transcriptomes for human respiratory epithelial, immune, and stromal cell types and subsets from an allergic inflammatory disease and mapped key mediators. They found striking differences between the epithelial compartments of the non-polyp and polyp cellular ecosystems, identifying and validating a global reduction of cellular subset diversity in polyps. Furthermore, they detected an aberrant basal epithelial stem cell differentiation trajectory in polyps and proposed cell-intrinsic, epigenetic, and cell-extrinsic factors that lock polyp basal progenitor cells into this uncommitted state. Finally, they functionally validated that basal cells ex vivo can retain intrinsic memory of allergic immune responses and tested the potential for clinical administration of antibody blockades of these signals to restore basal and secretory epithelial cell states in vivo. Overall, their work demonstrated that epithelial stem cells may contribute to the persistence of human disease by serving as repositories for allergic memories. In parallel, through local, national, and international collaborations, the Shalek lab pursued deep mechanistic inquiries across a diverse array of species and tissue isolates, defining healthy tissue compositions as well as deviations induced by different infections (e.g., malaria, leprosy), inflammatory diseases (e.g., ulcerative colitis), and cancers (e.g., pancreatic cancer, leukemia) with a view to novel therapeutic and prophylactic ends.

Matthew D. Shoulders

The Shoulders lab discovered that innate immune system escape by viruses such as influenza is made possible by the human host's protein-folding machinery promoting the folding of immune escape-competent viral protein variants that are otherwise incapable of folding on their own. This finding suggests new strategies to restrict viral evolution and potentiate host immune system function. The group also devised new high-throughput screening strategies for collagen secretion, leading to the discovery of a role for Hsp90 inhibitors in reducing excessive collagen secretion associated with fibrosis. In other work, the group developed methods for selective zinc depletion from complex biological media and new strategies for targeted mutagenesis in vivo, both of which have broad applications in biomedical research.

Daniel Suess

The Suess research group set up its laboratory and welcomed its first graduate students and postdoctoral fellows. Researchers began to uncover new reaction chemistry of

biological iron-sulfur clusters, particularly the active site of the enzyme nitrogenase. They also developed highly tunable, synthetic models of these clusters that allow for in-depth studies of their properties.

Yogesh Surendranath

The Surendranath group aims to use electricity to rearrange chemical bonds by manipulating interfacial reactivity at the molecular level. They have developed a new class of graphite-conjugated catalysts that combine the tunability of molecular catalysts with the rapid electron transfer properties of metallic extended solids. In addition, they have developed an electrochemical process for converting methane to derivatives of methanol, a versatile fuel and chemical intermediate. They also have uncovered a detailed mechanistic picture of how carbon dioxide is converted to hydrocarbon fuels.

Timothy M. Swager

Over the past year, new efforts in the Swager group focused on two areas. First, they developed novel detection methods for biological pathogens, including the Zika virus and *Salmonella* bacteria, using complex multiphase colloids. The colloids behave as dynamic lens materials that direct transmitted or emitted light in response to interactions with pathogens. These methods provide for ultra-sensitive and fast responses and are the basis of a start-up company that is launching in July 2018. Second, the group developed new magneto-optical materials that have large Faraday rotations in response to magnetic fields. These materials allow for detection of trace magnetic fields that can be used in the guidance systems of self-driving cars or to detect small electrical currents, potentially as small as those associated with brain activity. The new materials are semiconductive organic polymers having a helical structure in the solid state and ongoing efforts are targeting different helical semiconductive polymers.

Troy Van Voorhis

In the past year, the Van Voorhis group has been engaged in ground-breaking work on understanding energy and electron transfer at the nanoscale. In particular, they have developed new insights into fuel-forming RedOx catalysis at the surface of graphene, triplet energy transfer between molecules and colloidal quantum dots, and bimolecular processes in organic LEDs (light-emitting diodes).

Adam Willard

In AY2018, the Willard group made advances in developing and implementing theoretical models for simulating the electronic properties of molecular semiconductors such as organic electronic materials and quantum dot solids. They found that, contrary to previous expectations, a moderate amount of microscopic disorder can actually enhance the efficiency of organic-based solar cells. The group also made important advances in the understanding of water's interfacial molecular structure. These advances include the development of an analytical theory for predicting microscopic interfacial structure and a computational method for quantifying this structure in the context of molecular simulation.

Bin Zhang

The Zhang group developed a computational model to enable de novo prediction of three-dimensional genome organization using one-dimensional sequence information. The group's model directly demonstrates the sequence-structure relationship of the genome and will provide a greatly improved understanding of the driving force for genome folding.

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